Full wwPDB EM Validation Report ⓘ

Feb 1, 2023 – 07:20 pm GMT

PDB ID	:	7R45
EMDB ID	:	EMD-14272
Title	:	Bovine complex I in the presence of IM1761092, deactive class i (Composite map)
Authors	:	Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on	:	2022-02-08
Resolution	:	2.40 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

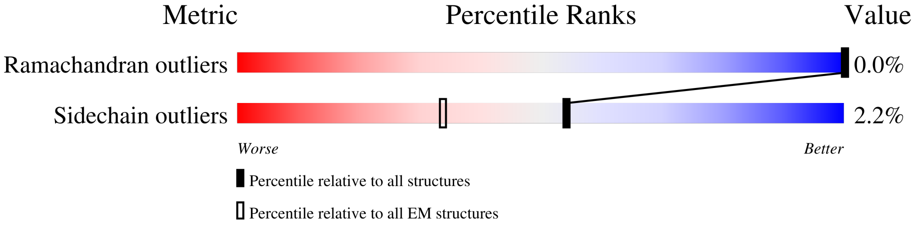
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

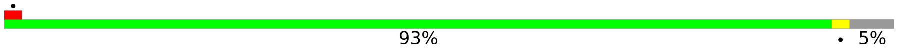
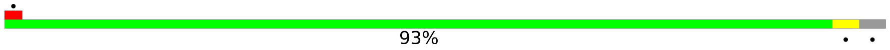
The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	216	
3	C	266	
4	D	463	
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	

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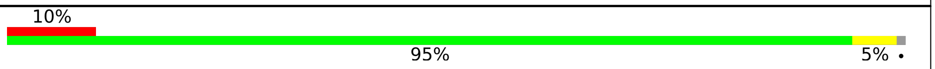
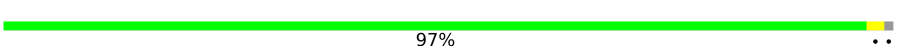
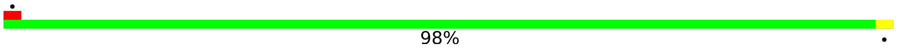
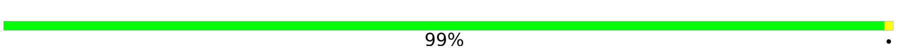
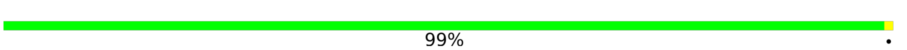
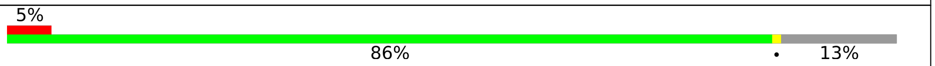
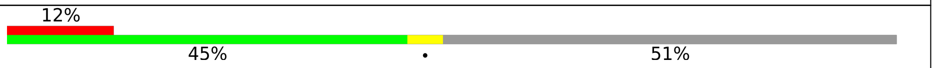
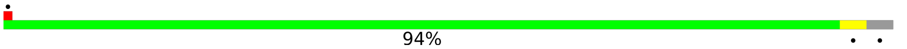
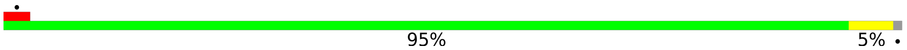
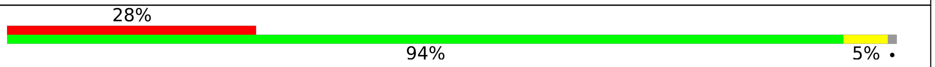
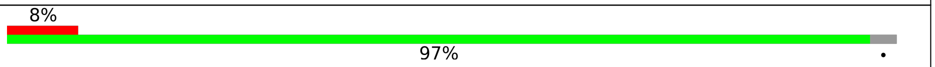
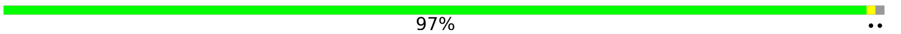
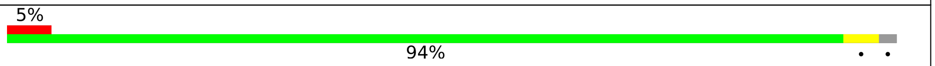
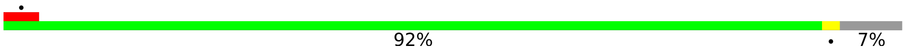
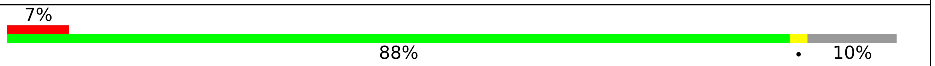
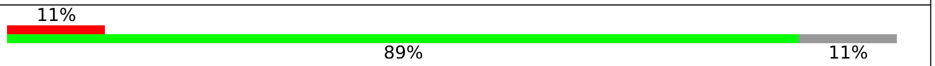
Mol	Chain	Length	Quality of chain
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	

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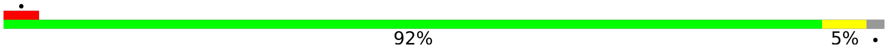
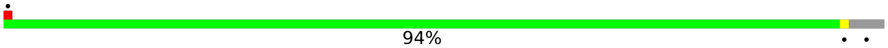
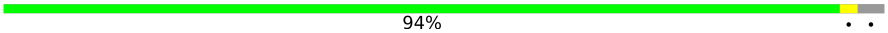
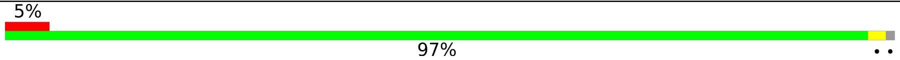
Mol	Chain	Length	Quality of chain
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition ⓘ

There are 60 unique types of molecules in this entry. The entry contains 68195 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	101	814	555	118	136	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	154	1230	786	220	210	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1714	1107	295	309	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	417	3363	2150	577	611	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1655	1057	277	311	10	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	430	3310	2085	591	614	20	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	688	5279	3307	920	1013	39	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	307	2425	1629	373	400	23	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	176	1414	889	243	270	12	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	174	1337	902	189	234	12	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	97	739	483	111	130	15	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	606	4786	3184	735	824	43	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3654	2436	570	609	39	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	347	2733	1817	416	457	43	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2589	1662	429	488	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	294	2342	1501	420	416	5	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	125	1016	641	181	191	3	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			730	448	137	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	84	Total	C	N	O	S	0	0
			681	439	100	137	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			911	589	154	165	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			971	622	180	165	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	140	1030	657	176	191	6	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	140	1146	737	200	200	9	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	69	561	361	103	92	5	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	82	646	422	108	114	2	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	c	48	405	268	69	68	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	112	934	613	157	161	3	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	95	799	506	150	137	6	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total 444	C 291	N 78	O 74	S 1	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	98	Total 824	C 529	N 137	O 154	S 4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total 1154	C 759	N 196	O 197	S 2	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	103	Total 884	C 584	N 149	O 150	S 1	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total 580	C 381	N 95	O 103	S 1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	79	Total 638	C 418	N 107	O 111	S 2	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	155	1304	844	213	239	8	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	m	126	1050	672	186	192	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	171	1487	952	272	256	7	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	121	1043	650	200	184	9	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	170	1435	900	265	262	8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	144	1201	773	215	209	4	0	0

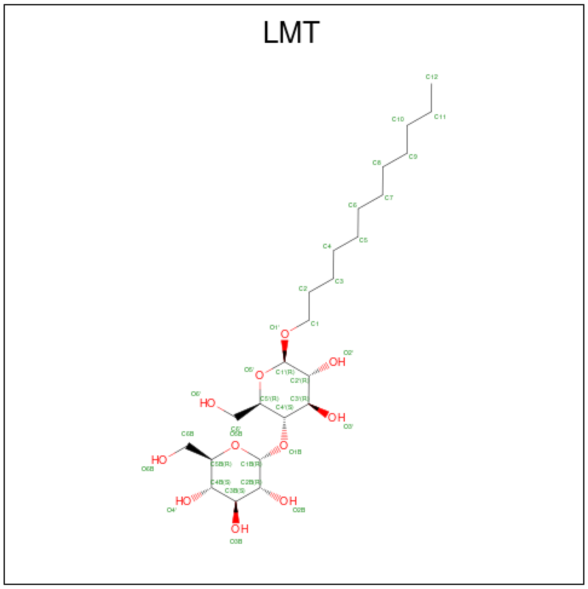
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	94	767	485	143	136	3	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	s	43	364	228	65	70	1	0	0

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	A	1	35	24	11	0
45	B	1	35	24	11	0
45	J	1	35	24	11	0
45	L	1	35	24	11	0
45	L	1	35	24	11	0
45	L	1	35	24	11	0
45	M	1	35	24	11	0

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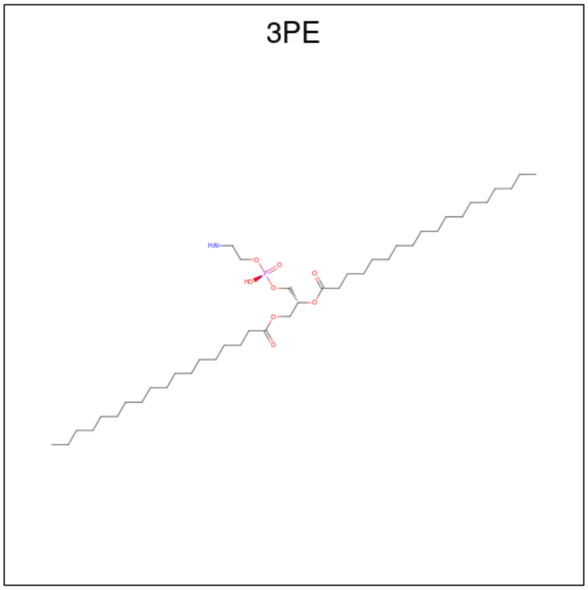
Mol	Chain	Residues	Atoms			AltConf
45	M	1	Total 35	C 24	O 11	0
45	M	1	Total 35	C 24	O 11	0
45	N	1	Total 35	C 24	O 11	0
45	f	1	Total 35	C 24	O 11	0
45	h	1	Total 35	C 24	O 11	0
45	l	1	Total 35	C 24	O 11	0

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total 36	C 26	N 1	O 8	P 1	0
46	H	1	Total 34	C 24	N 1	O 8	P 1	0
46	I	1	Total 51	C 41	N 1	O 8	P 1	0
46	J	1	Total 37	C 27	N 1	O 8	P 1	0
46	L	1	Total 48	C 38	N 1	O 8	P 1	0

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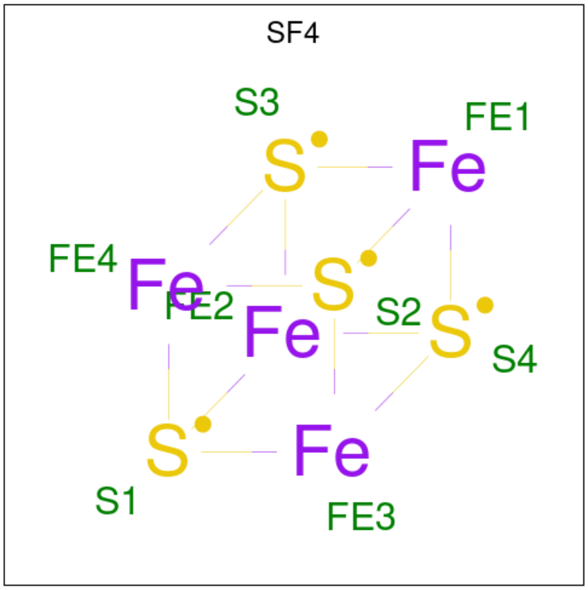
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	L	1	45	35	1	8	1	0
46	M	1	39	29	1	8	1	0
46	M	1	51	41	1	8	1	0
46	N	1	41	31	1	8	1	0
46	O	1	47	37	1	8	1	0
46	Y	1	35	25	1	8	1	0
46	b	1	39	29	1	8	1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	8	4	4	0
47	F	1	8	4	4	0
47	G	1	8	4	4	0
47	G	1	8	4	4	0

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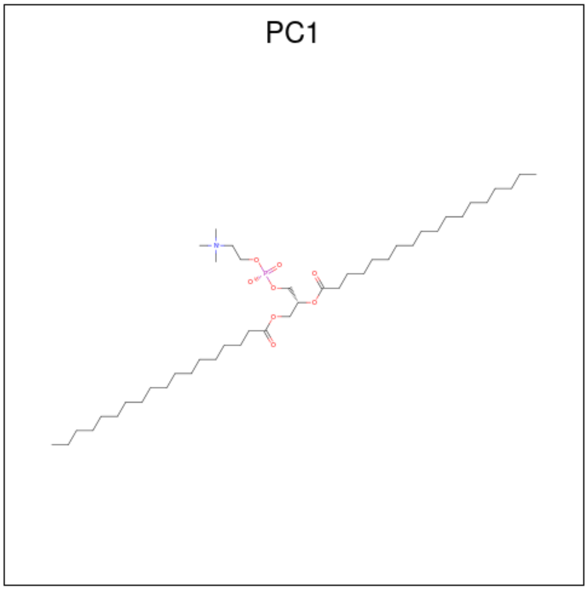
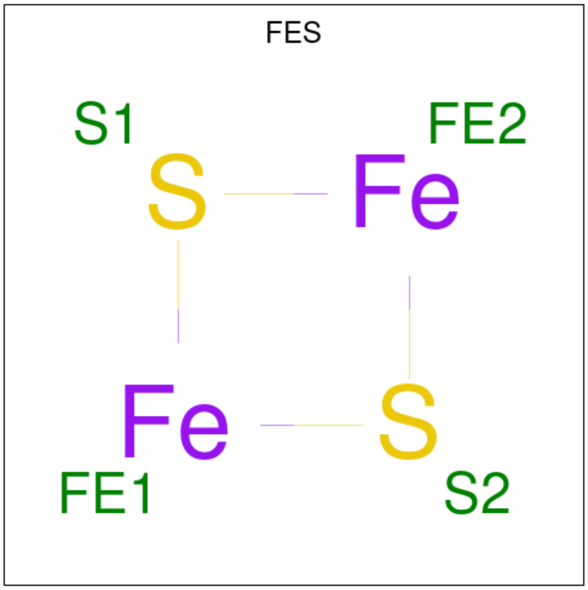
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total 8	Fe 4	S 4	0
47	I	1	Total 8	Fe 4	S 4	0

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



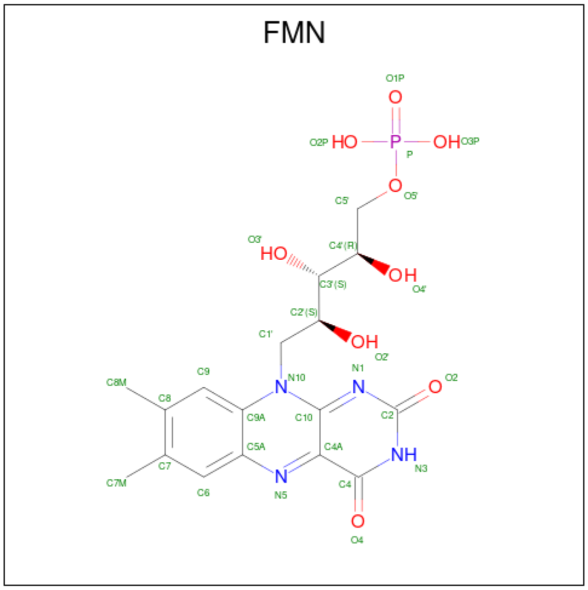
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total 35	C 25	N 1	O 8	P 1	0
48	M	1	Total 41	C 31	N 1	O 8	P 1	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
49	E	1	Total Fe S 4 2 2	0
49	G	1	Total Fe S 4 2 2	0

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

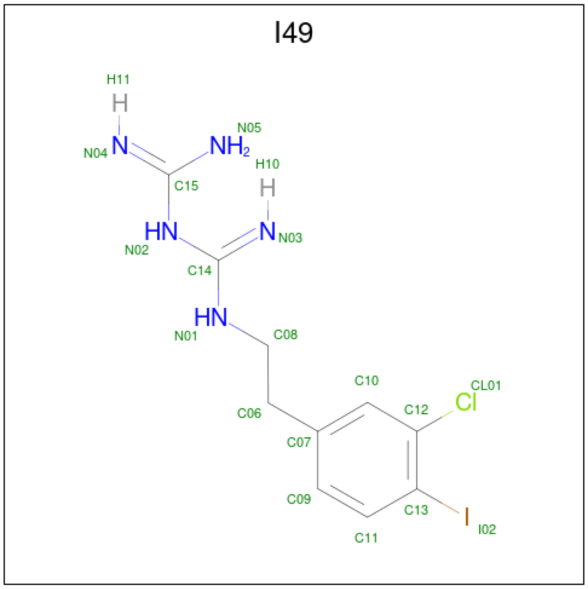


Mol	Chain	Residues	Atoms	AltConf
50	F	1	Total C N O P 31 17 4 9 1	0

- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).

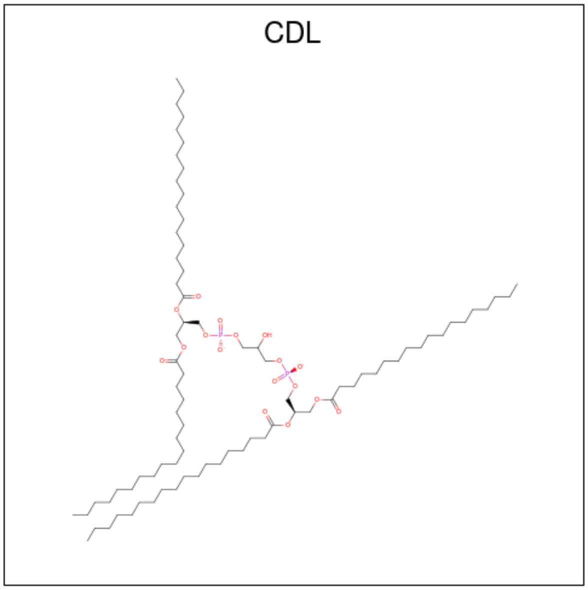
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
51	G	1	1	1	0

- Molecule 52 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (three-letter code: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



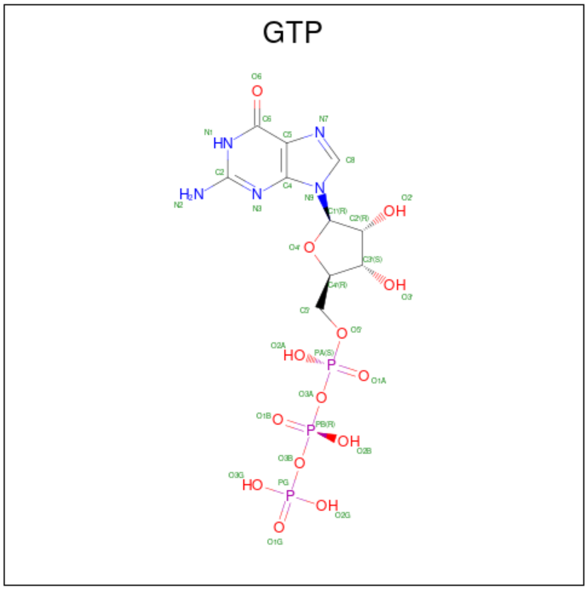
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	I	N	
52	H	1	17	10	1	1	5	0
52	N	1	17	10	1	1	5	0

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
53	K	1	Total 67	C 48	O 17	P 2	0
53	L	1	Total 100	C 81	O 17	P 2	0
53	X	1	Total 65	C 46	O 17	P 2	0
53	d	1	Total 65	C 46	O 17	P 2	0
53	h	1	Total 67	C 48	O 17	P 2	0
53	q	1	Total 76	C 57	O 17	P 2	0

- Molecule 54 is GUANOSINE-5’-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

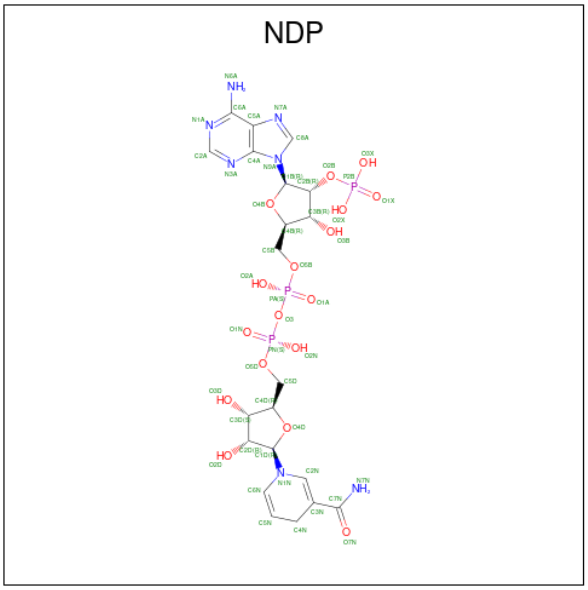


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	O	1	32	10	5	14	3	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
55	O	1	1	1	0

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

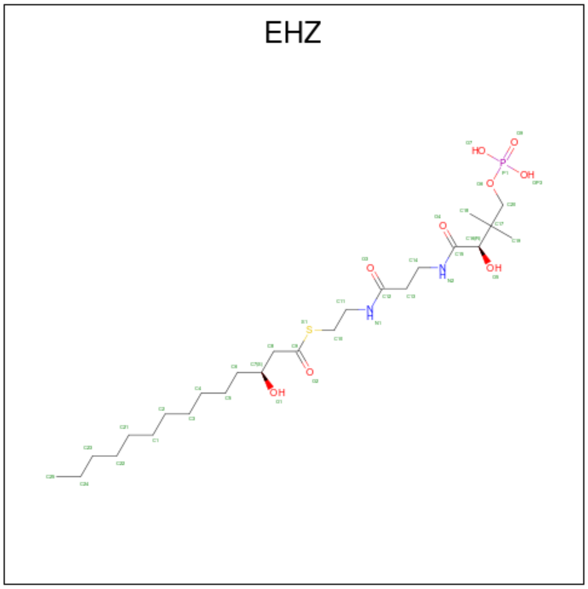


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	P	1	48	21	7	17	3	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

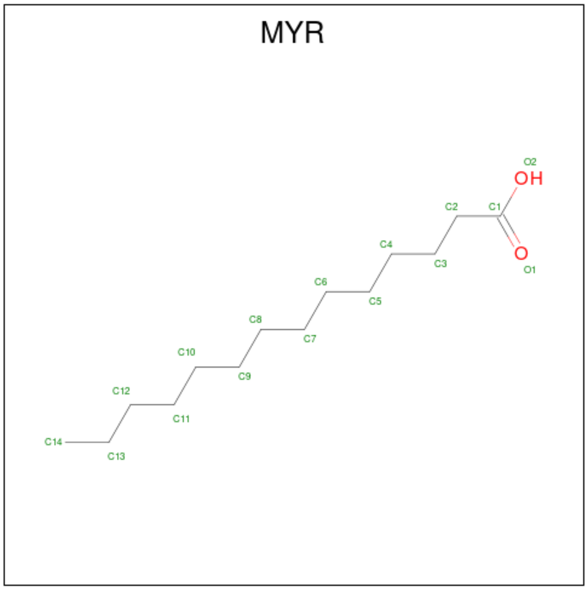
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	R	1	1	1	0

- Molecule 58 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
58	T	1	37	25	2	8	1	1	0
58	U	1	37	25	2	8	1	1	0

- Molecule 59 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	AltConf
59	o	1	Total C O 15 14 1	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	9	Total O 9 9	0
60	B	53	Total O 53 53	0
60	C	82	Total O 82 82	0
60	D	150	Total O 150 150	0
60	E	7	Total O 7 7	0
60	F	55	Total O 55 55	0
60	G	180	Total O 180 180	0
60	H	39	Total O 39 39	0
60	I	89	Total O 89 89	0
60	J	8	Total O 8 8	0
60	K	7	Total O 7 7	0

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Mol	Chain	Residues	Atoms	AltConf
60	L	61	Total O 61 61	0
60	M	63	Total O 63 63	0
60	N	39	Total O 39 39	0
60	O	11	Total O 11 11	0
60	P	44	Total O 44 44	0
60	Q	62	Total O 62 62	0
60	R	31	Total O 31 31	0
60	S	1	Total O 1 1	0
60	T	1	Total O 1 1	0
60	U	7	Total O 7 7	0
60	V	10	Total O 10 10	0
60	W	12	Total O 12 12	0
60	X	23	Total O 23 23	0
60	Y	2	Total O 2 2	0
60	Z	18	Total O 18 18	0
60	a	14	Total O 14 14	0
60	b	5	Total O 5 5	0
60	d	12	Total O 12 12	0
60	e	13	Total O 13 13	0
60	f	4	Total O 4 4	0
60	g	17	Total O 17 17	0

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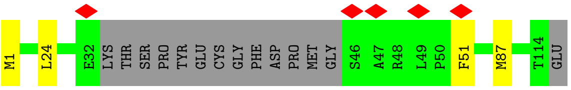
Mol	Chain	Residues	Atoms	AltConf
60	h	18	Total O 18 18	0
60	i	5	Total O 5 5	0
60	j	3	Total O 3 3	0
60	k	6	Total O 6 6	0
60	l	28	Total O 28 28	0
60	m	18	Total O 18 18	0
60	n	29	Total O 29 29	0
60	o	14	Total O 14 14	0
60	p	25	Total O 25 25	0
60	q	29	Total O 29 29	0
60	r	27	Total O 27 27	0
60	s	3	Total O 3 3	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

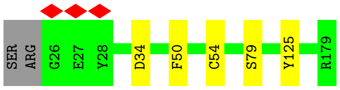
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



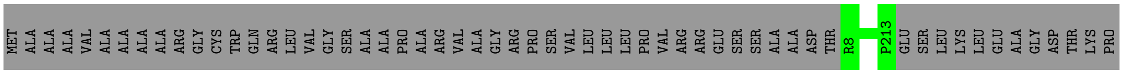
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:



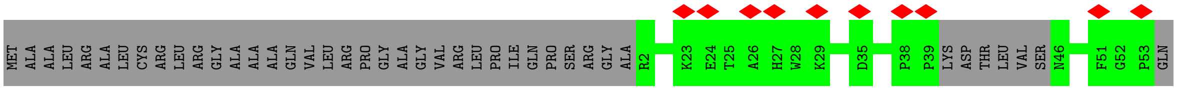
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

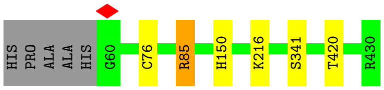
Chain C:



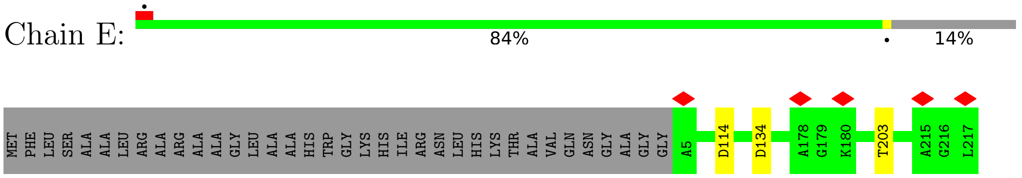
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:

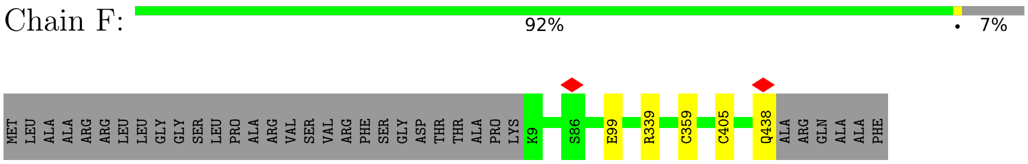




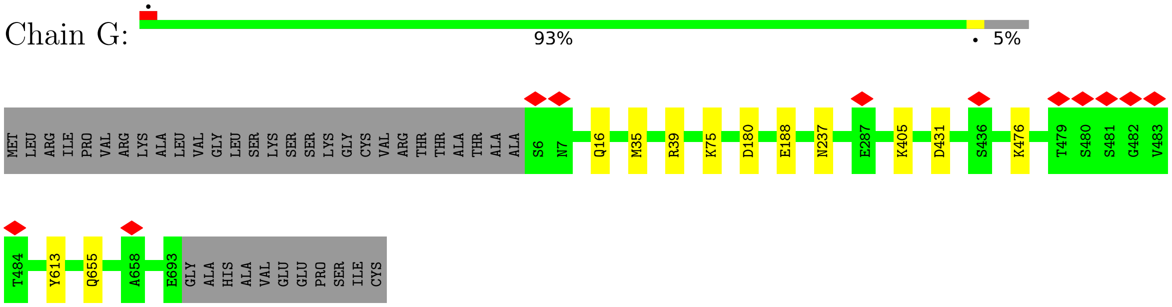
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



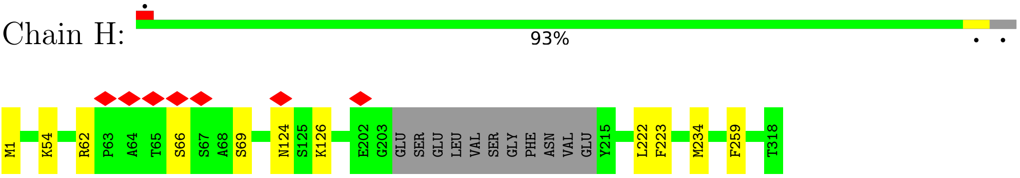
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



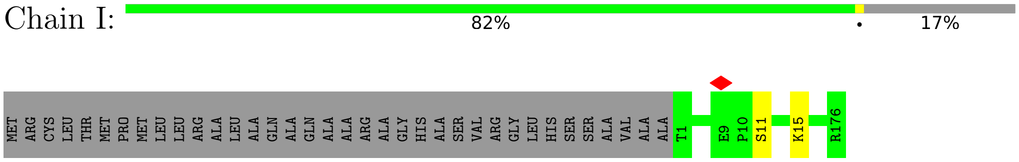
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



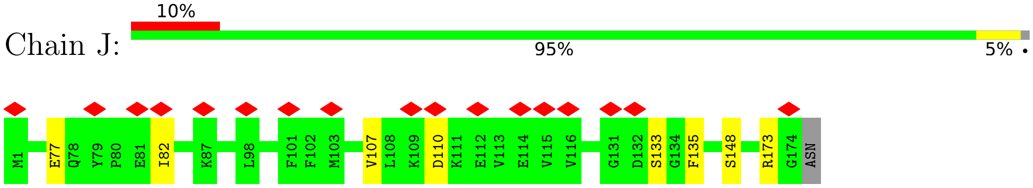
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



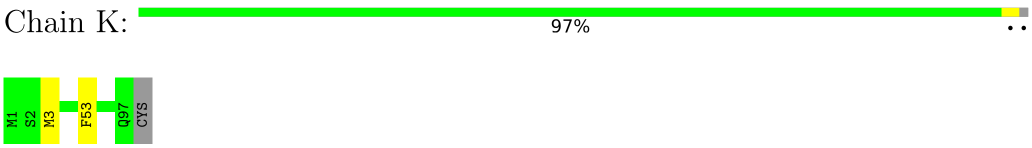
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



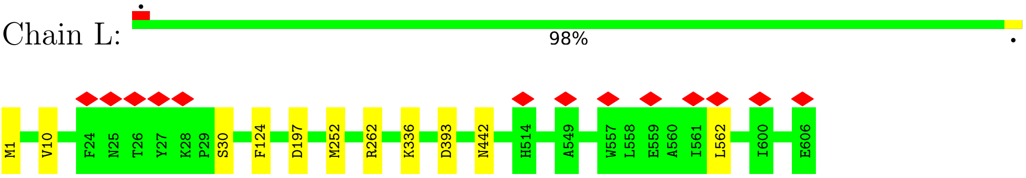
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



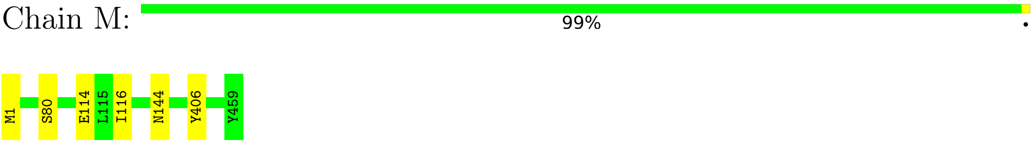
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



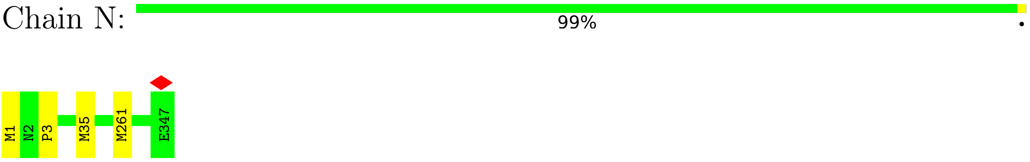
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



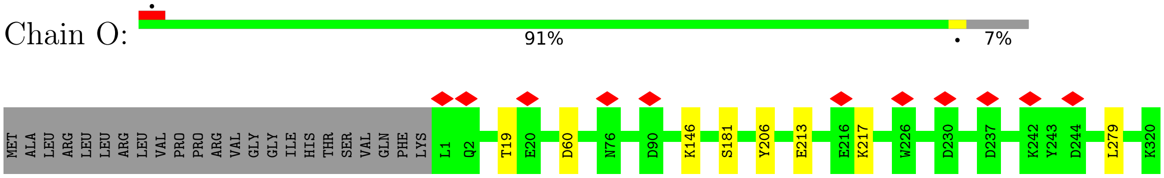
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



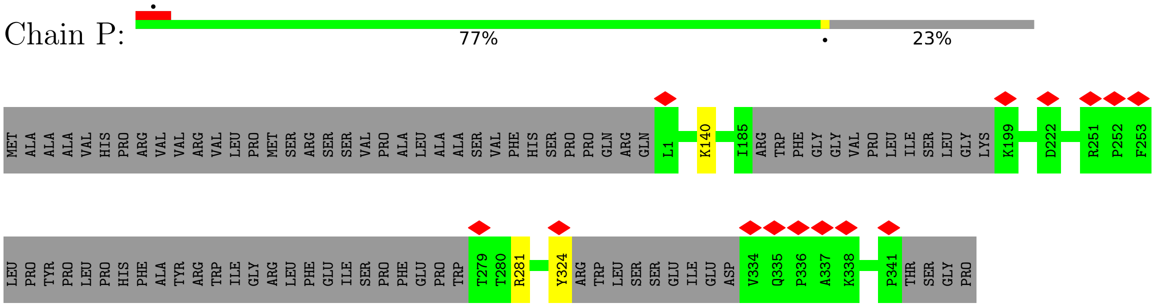
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



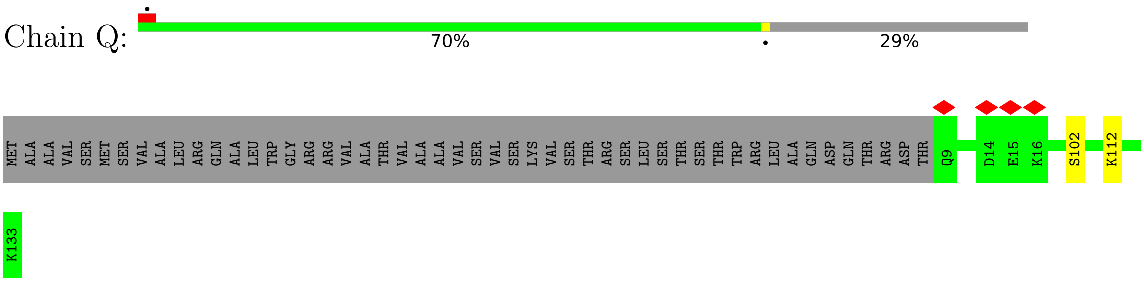
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



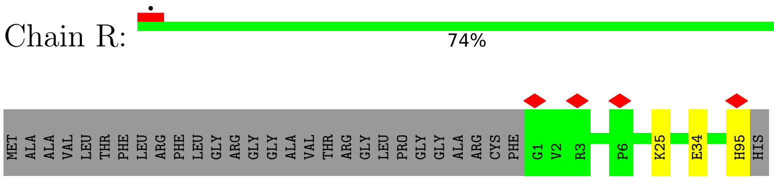
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



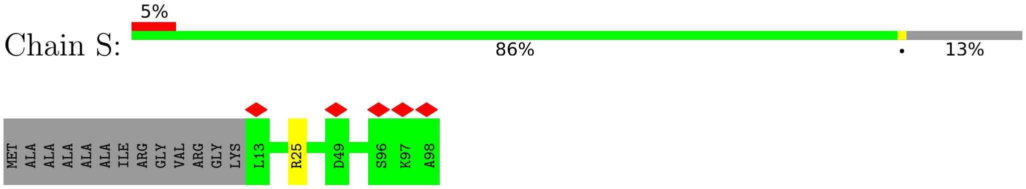
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



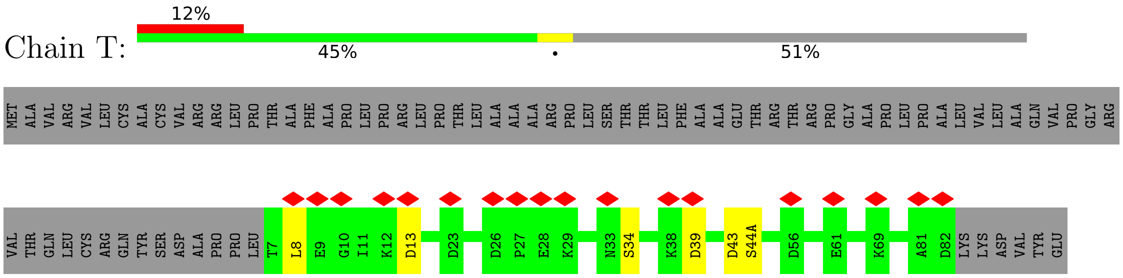
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



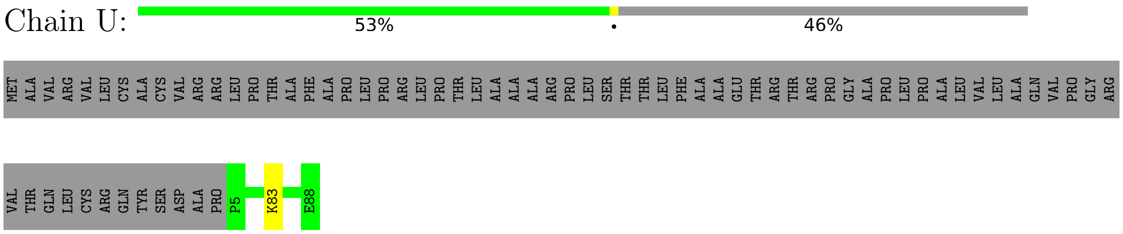
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



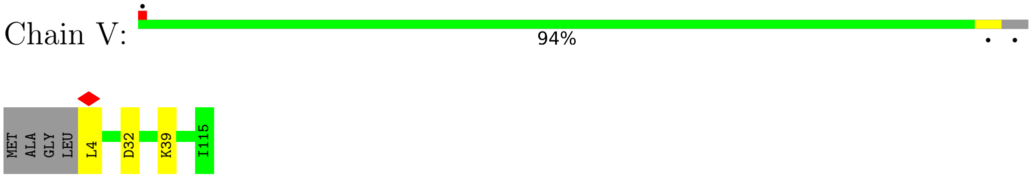
- Molecule 20: Acyl carrier protein, mitochondrial



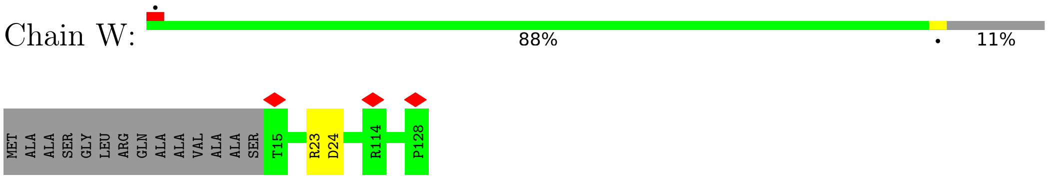
- Molecule 20: Acyl carrier protein, mitochondrial



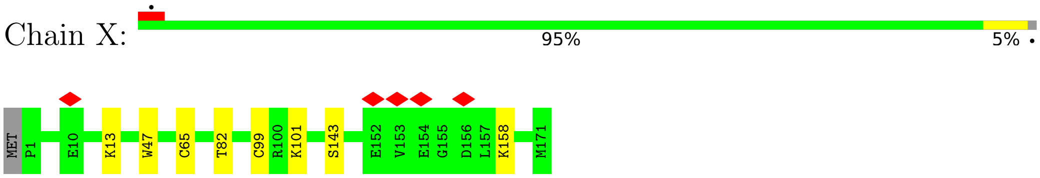
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



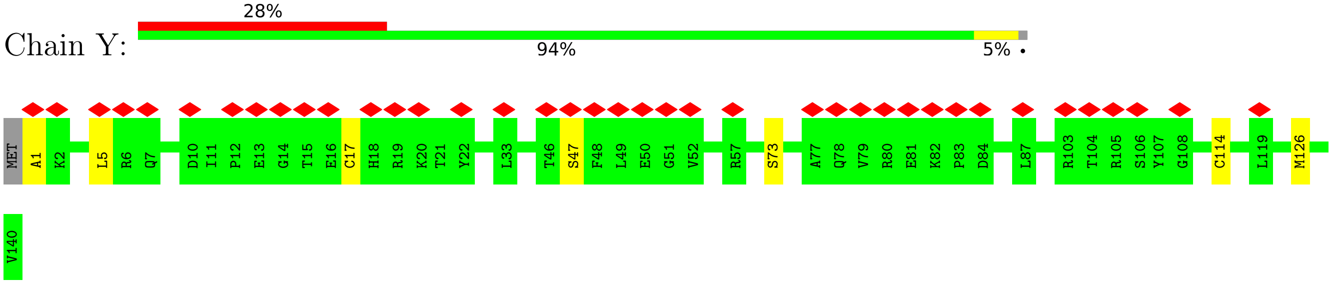
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



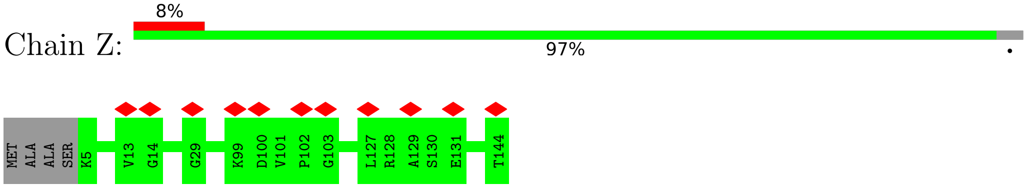
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



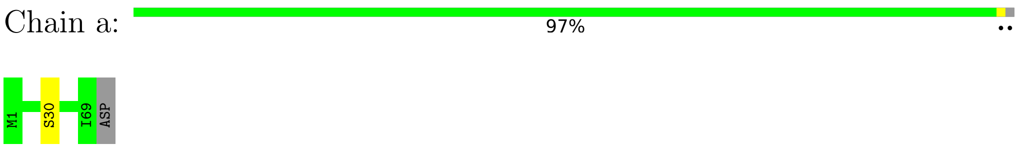
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



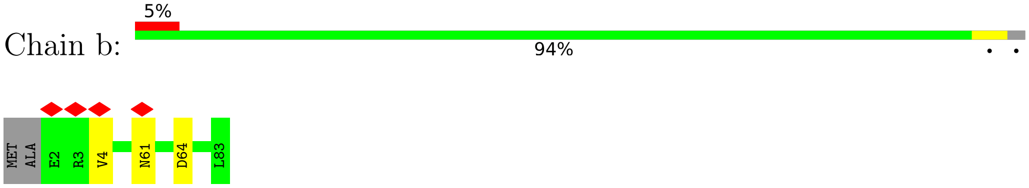
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

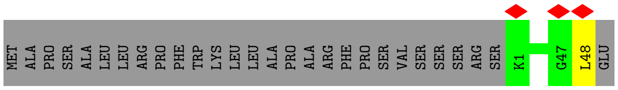


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



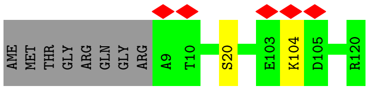
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:



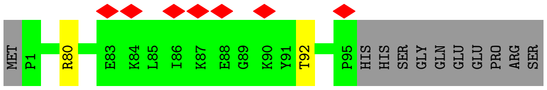
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:



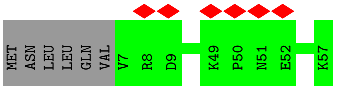
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



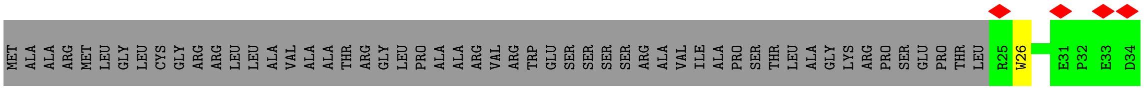
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

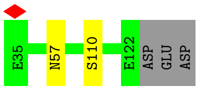
Chain f:



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

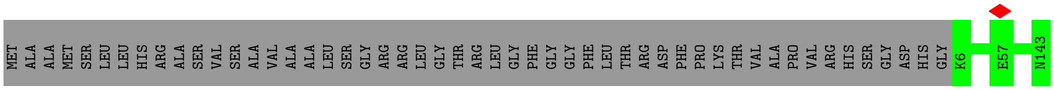
Chain g:





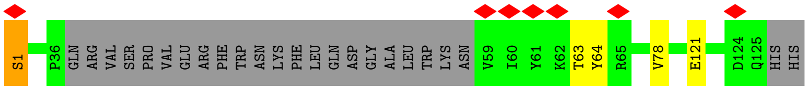
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:

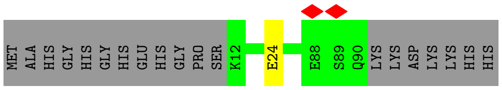


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:

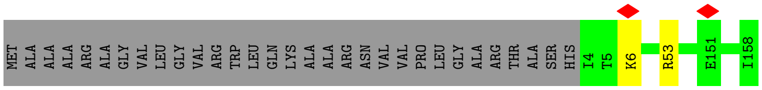
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



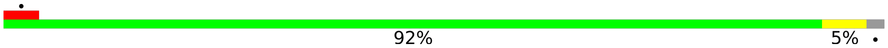
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

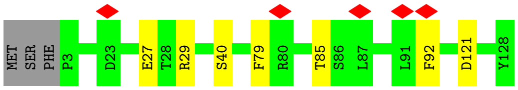
Chain l:



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

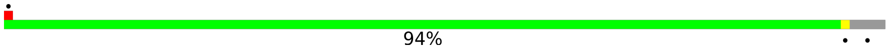
Chain m:

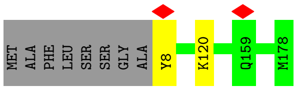




- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

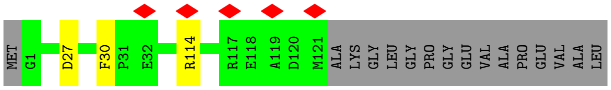
Chain n:





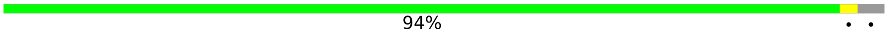
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

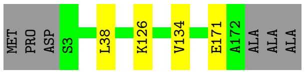
Chain o:



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

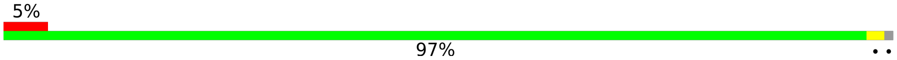
Chain p:

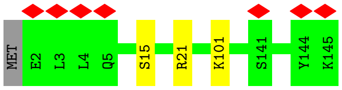




- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

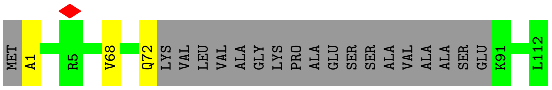
Chain q:





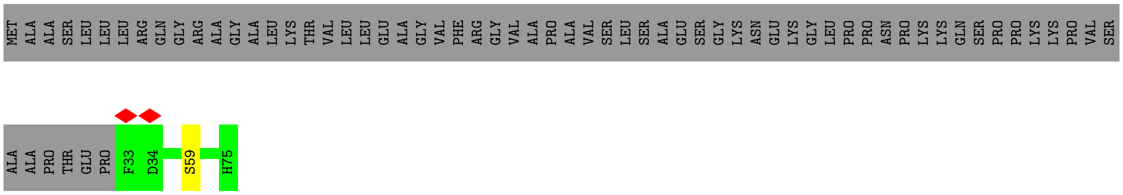
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68023	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	37.571	Depositor
Minimum map value	-16.074	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.063	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, K, SAC, SF4, EHZ, LMT, I49, MG, NDP, AYA, 3PE, PC1, FMN, MYR, GTP, FME, CDL, ZN, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/824	0.41	0/1128
2	B	0.39	0/1261	0.45	0/1706
3	C	0.35	0/1765	0.45	0/2403
4	D	0.34	0/3436	0.45	0/4652
5	E	0.33	0/1695	0.44	0/2307
6	F	0.32	0/3384	0.45	0/4573
7	G	0.32	0/5367	0.46	0/7274
8	H	0.34	0/2485	0.44	0/3395
9	I	0.36	0/1445	0.47	0/1956
10	J	0.32	0/1362	0.42	0/1848
11	K	0.30	0/739	0.43	0/1000
12	L	0.34	0/4903	0.43	0/6672
13	M	0.33	0/3738	0.42	0/5097
14	N	0.30	0/2792	0.44	0/3800
15	O	0.34	0/2651	0.41	0/3587
16	P	0.31	0/2395	0.45	0/3238
17	Q	0.32	0/1039	0.45	0/1404
18	R	0.35	0/742	0.45	0/999
19	S	0.29	0/702	0.47	0/945
20	T	0.29	0/621	0.40	0/837
20	U	0.38	0/692	0.40	0/932
21	V	0.30	0/931	0.38	0/1261
22	W	0.30	0/995	0.42	0/1337
23	X	0.32	0/1439	0.41	0/1942
24	Y	0.27	0/1042	0.41	0/1414
25	Z	0.32	0/1175	0.43	0/1584
26	a	0.34	0/576	0.44	0/775
27	b	0.31	0/667	0.42	0/916
28	c	0.32	0/418	0.39	0/567
29	d	0.36	0/964	0.41	0/1305
30	e	0.30	0/818	0.44	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.33	0/457	0.42	0/616
32	g	0.35	0/850	0.41	0/1154
33	h	0.34	0/1188	0.41	0/1607
34	i	0.37	0/904	0.42	0/1230
35	j	0.36	0/607	0.40	0/833
36	k	0.34	0/657	0.42	0/887
37	l	0.39	0/1358	0.41	0/1858
38	m	0.36	0/1076	0.45	0/1455
39	n	0.38	0/1540	0.40	0/2085
40	o	0.38	0/1068	0.41	0/1430
41	p	0.35	0/1468	0.42	0/1979
42	q	0.32	0/1242	0.48	1/1688 (0.1%)
43	r	0.33	0/780	0.45	0/1056
44	s	0.31	0/375	0.43	0/507
All	All	0.33	0/66633	0.43	1/90332 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
34	i	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	q	21	ARG	NE-CZ-NH2	5.21	122.91	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain
34	i	1	SAC	Mainchain

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
2	B	152/216 (70%)	145 (95%)	7 (5%)	0	100	100
3	C	204/266 (77%)	200 (98%)	4 (2%)	0	100	100
4	D	410/463 (89%)	401 (98%)	9 (2%)	0	100	100
5	E	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
6	F	428/464 (92%)	421 (98%)	7 (2%)	0	100	100
7	G	686/727 (94%)	669 (98%)	17 (2%)	0	100	100
8	H	303/318 (95%)	291 (96%)	12 (4%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	172/175 (98%)	159 (92%)	13 (8%)	0	100	100
11	K	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	583 (96%)	20 (3%)	1 (0%)	47	62
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	309 (97%)	9 (3%)	0	100	100
16	P	286/380 (75%)	281 (98%)	5 (2%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	93/124 (75%)	90 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	70 (95%)	4 (5%)	0	100	100
20	U	82/156 (53%)	82 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	V	110/116 (95%)	110 (100%)	0	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	138/144 (96%)	137 (99%)	1 (1%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
30	e	93/106 (88%)	91 (98%)	2 (2%)	0	100	100
31	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
32	g	96/154 (62%)	92 (96%)	4 (4%)	0	100	100
33	h	136/189 (72%)	136 (100%)	0	0	100	100
34	i	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	148 (97%)	5 (3%)	0	100	100
38	m	124/129 (96%)	118 (95%)	6 (5%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	119/137 (87%)	115 (97%)	4 (3%)	0	100	100
41	p	168/176 (96%)	168 (100%)	0	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	41/109 (38%)	39 (95%)	2 (5%)	0	100	100
All	All	7989/9212 (87%)	7805 (98%)	183 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/100 (88%)	85 (97%)	3 (3%)	37	56
2	B	130/175 (74%)	125 (96%)	5 (4%)	33	51
3	C	187/228 (82%)	187 (100%)	0	100	100
4	D	360/392 (92%)	355 (99%)	5 (1%)	67	82
5	E	183/205 (89%)	180 (98%)	3 (2%)	62	79
6	F	344/368 (94%)	339 (98%)	5 (2%)	65	80
7	G	578/608 (95%)	566 (98%)	12 (2%)	53	72
8	H	264/274 (96%)	254 (96%)	10 (4%)	33	51
9	I	151/175 (86%)	149 (99%)	2 (1%)	69	84
10	J	140/141 (99%)	132 (94%)	8 (6%)	20	33
11	K	84/85 (99%)	82 (98%)	2 (2%)	49	68
12	L	529/533 (99%)	520 (98%)	9 (2%)	60	78
13	M	412/412 (100%)	407 (99%)	5 (1%)	71	85
14	N	315/315 (100%)	312 (99%)	3 (1%)	76	88
15	O	283/303 (93%)	275 (97%)	8 (3%)	43	63
16	P	253/327 (77%)	250 (99%)	3 (1%)	71	85
17	Q	112/153 (73%)	110 (98%)	2 (2%)	59	76
18	R	78/97 (80%)	75 (96%)	3 (4%)	33	51
19	S	76/82 (93%)	75 (99%)	1 (1%)	69	84
20	T	70/135 (52%)	64 (91%)	6 (9%)	10	16
20	U	78/135 (58%)	77 (99%)	1 (1%)	69	84
21	V	100/102 (98%)	97 (97%)	3 (3%)	41	61
22	W	107/114 (94%)	105 (98%)	2 (2%)	57	75
23	X	154/155 (99%)	146 (95%)	8 (5%)	23	38
24	Y	101/102 (99%)	95 (94%)	6 (6%)	19	32
25	Z	119/121 (98%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	58/59 (98%)	57 (98%)	1 (2%)	60	78
27	b	71/72 (99%)	68 (96%)	3 (4%)	30	47
28	c	44/68 (65%)	43 (98%)	1 (2%)	50	70
29	d	100/105 (95%)	98 (98%)	2 (2%)	55	74
30	e	86/96 (90%)	84 (98%)	2 (2%)	50	70
31	f	48/54 (89%)	48 (100%)	0	100	100
32	g	89/131 (68%)	86 (97%)	3 (3%)	37	56
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	98/120 (82%)	94 (96%)	4 (4%)	30	48
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	61/76 (80%)	60 (98%)	1 (2%)	62	79
37	l	139/159 (87%)	137 (99%)	2 (1%)	67	82
38	m	112/115 (97%)	105 (94%)	7 (6%)	18	28
39	n	156/161 (97%)	154 (99%)	2 (1%)	69	84
40	o	110/120 (92%)	107 (97%)	3 (3%)	44	65
41	p	154/157 (98%)	150 (97%)	4 (3%)	46	66
42	q	130/131 (99%)	128 (98%)	2 (2%)	65	80
43	r	84/97 (87%)	82 (98%)	2 (2%)	49	68
44	s	42/92 (46%)	41 (98%)	1 (2%)	49	68
All	All	7060/7892 (90%)	6905 (98%)	155 (2%)	54	71

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	51	PHE
1	A	87	MET
2	B	34	ASP
2	B	50	PHE
2	B	54	CYS
2	B	79	SER
2	B	125	TYR
4	D	76	CYS
4	D	150	HIS
4	D	216	LYS

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Mol	Chain	Res	Type
4	D	341	SER
4	D	420	THR
5	E	114	ASP
5	E	134	ASP
5	E	203	THR
6	F	99	GLU
6	F	339	ARG
6	F	359	CYS
6	F	405	CYS
6	F	438	GLN
7	G	16	GLN
7	G	35	MET
7	G	39	ARG
7	G	75	LYS
7	G	180	ASP
7	G	188	GLU
7	G	237	ASN
7	G	405	LYS
7	G	431	ASP
7	G	476	LYS
7	G	613	TYR
7	G	655	GLN
8	H	54	LYS
8	H	62	ARG
8	H	66	SER
8	H	69	SER
8	H	124	ASN
8	H	126	LYS
8	H	222	LEU
8	H	223	PHE
8	H	234	MET
8	H	259	PHE
9	I	11	SER
9	I	15	LYS
10	J	77	GLU
10	J	82	ILE
10	J	107	VAL
10	J	110	ASP
10	J	133	SER
10	J	135	PHE
10	J	148	SER
10	J	173	ARG

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Mol	Chain	Res	Type
11	K	3	MET
11	K	53	PHE
12	L	10	VAL
12	L	30	SER
12	L	124	PHE
12	L	197	ASP
12	L	252	MET
12	L	262	ARG
12	L	336	LYS
12	L	393	ASP
12	L	442	ASN
13	M	80	SER
13	M	114	GLU
13	M	116	ILE
13	M	144	ASN
13	M	406	TYR
14	N	3	PRO
14	N	35	MET
14	N	261	MET
15	O	19	THR
15	O	60	ASP
15	O	146	LYS
15	O	181	SER
15	O	206	TYR
15	O	213	GLU
15	O	217	LYS
15	O	279	LEU
16	P	140	LYS
16	P	281	ARG
16	P	324	TYR
17	Q	102	SER
17	Q	112	LYS
18	R	25	LYS
18	R	34	GLU
18	R	95	HIS
19	S	25	ARG
20	T	8	LEU
20	T	13	ASP
20	T	34	SER
20	T	39	ASP
20	T	43	ASP
20	T	44(A)	SER

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Mol	Chain	Res	Type
20	U	83	LYS
21	V	4	LEU
21	V	32	ASP
21	V	39	LYS
22	W	23	ARG
22	W	24	ASP
23	X	13	LYS
23	X	47	TRP
23	X	65	CYS
23	X	82	THR
23	X	99	CYS
23	X	101	LYS
23	X	143	SER
23	X	158	LYS
24	Y	5	LEU
24	Y	17	CYS
24	Y	47	SER
24	Y	73	SER
24	Y	114	CYS
24	Y	126	MET
26	a	30	SER
27	b	4	VAL
27	b	61	ASN
27	b	64	ASP
28	c	48	LEU
29	d	20	SER
29	d	104	LYS
30	e	80	ARG
30	e	92	THR
32	g	26	TRP
32	g	57	ASN
32	g	110	SER
34	i	63	THR
34	i	64	TYR
34	i	78	VAL
34	i	121	GLU
36	k	24	GLU
37	l	6	LYS
37	l	53	ARG
38	m	27	GLU
38	m	29	ARG
38	m	40	SER

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Mol	Chain	Res	Type
38	m	79	PHE
38	m	85	THR
38	m	92	PHE
38	m	121	ASP
39	n	8	TYR
39	n	120	LYS
40	o	27	ASP
40	o	30	PHE
40	o	114	ARG
41	p	38	LEU
41	p	126	LYS
41	p	134	VAL
41	p	171	GLU
42	q	15	SER
42	q	101	LYS
43	r	68	VAL
43	r	72	GLN
44	s	59	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	435	GLN
15	O	190	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	2MR	D	85	4	10,12,13	2.63	4 (40%)	5,13,15	1.14	1 (20%)
14	FME	N	1	14	8,9,10	0.95	0	7,9,11	1.07	1 (14%)
24	AYA	Y	1	24	6,7,8	1.81	2 (33%)	5,8,10	1.11	1 (20%)
43	AYA	r	1	43	6,7,8	1.80	2 (33%)	5,8,10	1.42	1 (20%)
11	FME	K	1	11	8,9,10	0.90	0	7,9,11	0.93	0
34	SAC	i	1	34	7,8,9	1.80	1 (14%)	8,9,11	1.90	1 (12%)
1	FME	A	1	1	8,9,10	1.00	1 (12%)	7,9,11	0.78	0
8	FME	H	1	8	8,9,10	0.92	0	7,9,11	1.14	1 (14%)
10	FME	J	1	10	8,9,10	0.90	0	7,9,11	0.83	0
12	FME	L	1	12	8,9,10	0.91	0	7,9,11	1.05	1 (14%)
13	FME	M	1	13	8,9,10	0.98	1 (12%)	7,9,11	1.08	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MR	D	85	4	-	0/10/13/15	-
14	FME	N	1	14	-	2/7/9/11	-
24	AYA	Y	1	24	-	1/4/6/8	-
43	AYA	r	1	43	-	0/4/6/8	-
11	FME	K	1	11	-	0/7/9/11	-
34	SAC	i	1	34	-	1/7/8/10	-
1	FME	A	1	1	-	2/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.97	1.44	1.33
4	D	85	2MR	CZ-NE	4.61	1.44	1.34
34	i	1	SAC	O-C	4.12	1.36	1.19
4	D	85	2MR	O-C	3.87	1.35	1.19
24	Y	1	AYA	CT-N	3.32	1.45	1.34
43	r	1	AYA	CT-N	3.19	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	r	1	AYA	OT-CT	-2.06	1.18	1.23
4	D	85	2MR	CQ1-NH1	-2.06	1.42	1.46
13	M	1	FME	CA-N	-2.04	1.43	1.46
24	Y	1	AYA	OT-CT	-2.03	1.18	1.23
1	A	1	FME	CA-N	-2.01	1.43	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	O-C-CA	-4.71	112.44	124.78
43	r	1	AYA	CM-CT-N	2.45	120.25	116.10
13	M	1	FME	C-CA-N	2.34	113.95	109.73
8	H	1	FME	C-CA-N	2.33	113.93	109.73
4	D	85	2MR	NE-CZ-NH2	-2.28	117.39	119.48
14	N	1	FME	C-CA-N	2.18	113.67	109.73
24	Y	1	AYA	CM-CT-N	2.05	119.56	116.10
12	L	1	FME	C-CA-N	2.04	113.41	109.73

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	N-CA-CB-CG
34	i	1	SAC	C-CA-CB-OG
12	L	1	FME	CA-CB-CG-SD
8	H	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
24	Y	1	AYA	C-CA-N-CT
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 52 ligands modelled in this entry, 3 are monoatomic - leaving 49 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	LMT	l	201	-	36,36,36	1.18	3 (8%)	47,47,47	0.94	0
52	I49	H	602	-	15,17,17	1.53	2 (13%)	21,22,22	2.65	7 (33%)
45	LMT	M	606	-	36,36,36	1.28	5 (13%)	47,47,47	1.12	4 (8%)
45	LMT	A	301	-	36,36,36	1.22	4 (11%)	47,47,47	0.79	1 (2%)
53	CDL	L	704	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
58	EHZ	T	101	20	29,36,37	1.66	5 (17%)	35,44,47	1.40	3 (8%)
45	LMT	h	1002	-	36,36,36	1.15	2 (5%)	47,47,47	1.10	4 (8%)
45	LMT	L	706	-	36,36,36	1.17	2 (5%)	47,47,47	0.92	1 (2%)
53	CDL	K	401	-	66,66,99	1.06	8 (12%)	72,78,111	1.06	4 (5%)
54	GTP	O	1202	55	26,34,34	2.90	10 (38%)	32,54,54	1.74	11 (34%)
53	CDL	q	201	-	75,75,99	0.99	7 (9%)	81,87,111	1.06	4 (4%)
47	SF4	G	801	7	0,12,12	-	-	-		
46	3PE	b	901	-	38,38,50	0.95	4 (10%)	41,43,55	1.11	2 (4%)
49	FES	E	301	5	0,4,4	-	-	-		
46	3PE	O	1201	-	46,46,50	0.91	4 (8%)	49,51,55	1.04	2 (4%)
56	NDP	P	501	-	45,52,52	2.17	5 (11%)	53,80,80	1.69	11 (20%)
47	SF4	B	201	2	0,12,12	-	-	-		
46	3PE	I	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.02	2 (3%)
45	LMT	M	602	-	36,36,36	1.16	3 (8%)	47,47,47	1.25	3 (6%)
58	EHZ	U	101	20	29,36,37	1.69	6 (20%)	35,44,47	1.46	4 (11%)
53	CDL	h	1001	-	66,66,99	1.05	6 (9%)	72,78,111	1.18	4 (5%)
45	LMT	B	202	-	36,36,36	1.18	2 (5%)	47,47,47	0.85	1 (2%)
45	LMT	J	402	-	36,36,36	1.21	3 (8%)	47,47,47	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
53	CDL	X	1701	-	64,64,99	1.01	6 (9%)	68,75,111	1.12	4 (5%)
47	SF4	F	502	6	0,12,12	-	-	-		
46	3PE	M	603	-	50,50,50	0.86	4 (8%)	53,55,55	1.10	2 (3%)
53	CDL	d	201	-	64,64,99	1.07	8 (12%)	70,76,111	1.13	4 (5%)
46	3PE	A	302	-	35,35,50	1.02	4 (11%)	38,40,55	1.12	2 (5%)
45	LMT	L	705	-	36,36,36	1.16	3 (8%)	47,47,47	1.02	3 (6%)
45	LMT	L	702	-	36,36,36	1.17	3 (8%)	47,47,47	1.13	4 (8%)
48	PC1	M	604	-	40,40,53	1.08	4 (10%)	46,48,61	1.01	2 (4%)
48	PC1	B	203	-	34,34,53	1.15	4 (11%)	40,42,61	1.09	2 (5%)
50	FMN	F	501	-	33,33,33	1.11	3 (9%)	48,50,50	1.28	6 (12%)
45	LMT	M	605	-	36,36,36	1.17	3 (8%)	47,47,47	0.96	1 (2%)
52	I49	N	503	-	15,17,17	1.56	2 (13%)	21,22,22	1.75	5 (23%)
47	SF4	G	802	7	0,12,12	-	-	-		
59	MYR	o	201	40	14,14,15	0.91	0	13,13,15	0.68	0
49	FES	G	803	7	0,4,4	-	-	-		
45	LMT	N	501	-	36,36,36	1.17	3 (8%)	47,47,47	0.89	1 (2%)
47	SF4	I	203	9	0,12,12	-	-	-		
46	3PE	J	401	-	36,36,50	1.00	4 (11%)	39,41,55	1.11	2 (5%)
46	3PE	M	601	-	38,38,50	0.96	4 (10%)	41,43,55	1.10	2 (4%)
46	3PE	L	703	-	44,44,50	0.91	3 (6%)	47,49,55	1.16	2 (4%)
46	3PE	Y	401	-	34,34,50	1.03	4 (11%)	37,39,55	1.15	2 (5%)
46	3PE	L	701	-	47,47,50	0.89	2 (4%)	50,52,55	1.03	2 (4%)
46	3PE	N	502	-	40,40,50	0.95	4 (10%)	43,45,55	1.16	2 (4%)
45	LMT	f	1901	-	36,36,36	1.18	2 (5%)	47,47,47	0.94	3 (6%)
46	3PE	H	601	-	33,33,50	1.39	4 (12%)	34,37,55	1.13	2 (5%)
47	SF4	I	202	9	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	l	201	-	-	10/21/61/61	0/2/2/2
52	I49	H	602	-	-	5/10/10/10	0/1/1/1
45	LMT	M	606	-	-	9/21/61/61	0/2/2/2
45	LMT	A	301	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	L	704	-	-	44/110/110/110	-
58	EHZ	T	101	20	-	11/42/44/45	-
45	LMT	h	1002	-	-	4/21/61/61	0/2/2/2
45	LMT	L	706	-	-	11/21/61/61	0/2/2/2
53	CDL	K	401	-	-	26/77/77/110	-
54	GTP	O	1202	55	-	5/18/38/38	0/3/3/3
53	CDL	q	201	-	-	37/86/86/110	-
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	b	901	-	-	22/42/42/54	-
49	FES	E	301	5	-	-	0/1/1/1
46	3PE	O	1201	-	-	23/50/50/54	-
56	NDP	P	501	-	-	7/30/77/77	0/5/5/5
47	SF4	B	201	2	-	-	0/6/5/5
46	3PE	I	201	-	-	20/54/54/54	-
45	LMT	M	602	-	-	4/21/61/61	0/2/2/2
58	EHZ	U	101	20	-	8/42/44/45	-
53	CDL	h	1001	-	-	33/77/77/110	-
45	LMT	B	202	-	-	5/21/61/61	0/2/2/2
45	LMT	J	402	-	-	7/21/61/61	0/2/2/2
53	CDL	X	1701	-	-	35/74/74/110	-
47	SF4	F	502	6	-	-	0/6/5/5
46	3PE	M	603	-	-	26/54/54/54	-
53	CDL	d	201	-	-	35/75/75/110	-
46	3PE	A	302	-	-	14/39/39/54	-
45	LMT	L	705	-	-	8/21/61/61	0/2/2/2
45	LMT	L	702	-	-	3/21/61/61	0/2/2/2
48	PC1	M	604	-	-	14/44/44/57	-
48	PC1	B	203	-	-	12/38/38/57	-
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
45	LMT	M	605	-	-	9/21/61/61	0/2/2/2
52	I49	N	503	-	-	3/10/10/10	0/1/1/1
59	MYR	o	201	40	-	6/11/12/13	-
47	SF4	G	802	7	-	-	0/6/5/5
49	FES	G	803	7	-	-	0/1/1/1
45	LMT	N	501	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	I	203	9	-	-	0/6/5/5
46	3PE	J	401	-	-	23/40/40/54	-
46	3PE	M	601	-	-	17/42/42/54	-
46	3PE	L	703	-	-	20/48/48/54	-
46	3PE	Y	401	-	-	16/38/38/54	-
46	3PE	L	701	-	-	21/51/51/54	-
46	3PE	N	502	-	-	22/44/44/54	-
45	LMT	f	1901	-	-	12/21/61/61	0/2/2/2
46	3PE	H	601	-	-	15/36/36/54	-
47	SF4	I	202	9	-	-	0/6/5/5

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.14	1.82	1.59
54	O	1202	GTP	O6-C6	8.17	1.39	1.23
46	H	601	3PE	O21-C2	-5.60	1.40	1.46
58	U	101	EHZ	C15-N2	5.36	1.45	1.33
54	O	1202	GTP	O4'-C1'	5.34	1.48	1.41
58	T	101	EHZ	C15-N2	5.21	1.45	1.33
58	T	101	EHZ	C12-N1	5.07	1.44	1.33
58	U	101	EHZ	C12-N1	5.06	1.44	1.33
52	N	503	I49	C15-N02	-4.81	1.31	1.37
54	O	1202	GTP	C2-N1	4.72	1.49	1.37
52	H	602	I49	C15-N02	-4.63	1.31	1.37
54	O	1202	GTP	C2-N3	4.57	1.44	1.33
54	O	1202	GTP	C2-N2	4.57	1.45	1.34
50	F	501	FMN	C4A-N5	3.61	1.37	1.30
45	M	606	LMT	O5'-C1'	3.61	1.51	1.41
45	J	402	LMT	O5B-C1B	3.56	1.50	1.41
45	N	501	LMT	O5B-C1B	3.49	1.50	1.41
45	M	605	LMT	O5B-C1B	3.47	1.50	1.41
45	f	1901	LMT	O5B-C1B	3.47	1.50	1.41
45	M	606	LMT	O5B-C1B	3.46	1.50	1.41
45	B	202	LMT	O5B-C1B	3.41	1.50	1.41
45	A	301	LMT	O5B-C1B	3.40	1.50	1.41
45	l	201	LMT	O5B-C1B	3.39	1.50	1.41
45	L	705	LMT	O5B-C1B	3.36	1.50	1.41
45	M	602	LMT	O5B-C1B	3.34	1.50	1.41
54	O	1202	GTP	C2'-C1'	-3.28	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	706	LMT	O5B-C1B	3.25	1.50	1.41
56	P	501	NDP	O2B-C2B	-3.21	1.32	1.44
45	A	301	LMT	O5'-C1'	3.21	1.50	1.41
45	J	402	LMT	O5'-C1'	3.18	1.50	1.41
56	P	501	NDP	PN-O5D	3.18	1.72	1.59
45	h	1002	LMT	O5B-C1B	3.16	1.49	1.41
45	M	605	LMT	O5'-C1'	3.15	1.49	1.41
54	O	1202	GTP	C5-C6	-3.14	1.41	1.47
52	H	602	I49	C14-N03	3.14	1.38	1.29
52	N	503	I49	C14-N03	3.13	1.38	1.29
46	H	601	3PE	O21-C21	3.12	1.40	1.33
45	L	702	LMT	O5B-C1B	3.11	1.49	1.41
45	L	706	LMT	O5'-C1'	3.11	1.49	1.41
45	l	201	LMT	O5'-C1'	3.01	1.49	1.41
45	f	1901	LMT	O5'-C1'	3.01	1.49	1.41
45	N	501	LMT	O5'-C1'	2.99	1.49	1.41
45	M	602	LMT	O5'-C1'	2.99	1.49	1.41
45	L	705	LMT	O5'-C1'	2.95	1.49	1.41
45	L	702	LMT	O5'-C1'	2.90	1.49	1.41
46	L	701	3PE	O21-C2	-2.87	1.39	1.46
45	B	202	LMT	O5'-C1'	2.85	1.49	1.41
53	h	1001	CDL	OA6-CA4	-2.80	1.39	1.46
45	h	1002	LMT	O5'-C1'	2.79	1.48	1.41
46	L	701	3PE	O31-C3	-2.67	1.39	1.45
53	L	704	CDL	OB6-CB4	-2.66	1.39	1.46
46	L	703	3PE	O21-C2	-2.66	1.39	1.46
53	q	201	CDL	OA6-CA4	-2.65	1.40	1.46
53	K	401	CDL	OA6-CA4	-2.65	1.40	1.46
53	X	1701	CDL	OA6-CA4	-2.64	1.40	1.46
46	O	1201	3PE	O21-C2	-2.63	1.40	1.46
53	h	1001	CDL	OB6-CB4	-2.61	1.40	1.46
58	T	101	EHZ	O4-C15	-2.60	1.18	1.23
58	U	101	EHZ	O4-C15	-2.58	1.18	1.23
46	A	302	3PE	O21-C2	-2.57	1.40	1.46
53	q	201	CDL	OB6-CB4	-2.57	1.40	1.46
53	d	201	CDL	OA6-CA4	-2.57	1.40	1.46
46	M	603	3PE	O21-C2	-2.57	1.40	1.46
53	X	1701	CDL	OB6-CB4	-2.55	1.40	1.46
46	L	703	3PE	O31-C3	-2.53	1.39	1.45
48	M	604	PC1	O21-C2	-2.53	1.40	1.46
46	Y	401	3PE	O21-C2	-2.52	1.40	1.46
46	I	201	3PE	O31-C3	-2.52	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	J	401	3PE	O21-C2	-2.52	1.40	1.46
46	I	201	3PE	O21-C2	-2.52	1.40	1.46
46	b	901	3PE	O21-C2	-2.52	1.40	1.46
46	N	502	3PE	O21-C2	-2.50	1.40	1.46
46	N	502	3PE	O31-C3	-2.50	1.39	1.45
53	K	401	CDL	OB8-CB7	2.50	1.40	1.33
53	K	401	CDL	OB6-CB4	-2.49	1.40	1.46
53	L	704	CDL	OA8-CA7	2.46	1.40	1.33
48	B	203	PC1	O21-C2	-2.45	1.40	1.46
53	d	201	CDL	OB8-CB7	2.44	1.40	1.33
53	h	1001	CDL	OB8-CB6	-2.44	1.39	1.45
53	d	201	CDL	OB6-CB4	-2.44	1.40	1.46
53	q	201	CDL	OB8-CB7	2.43	1.40	1.33
54	O	1202	GTP	C2'-C3'	-2.42	1.46	1.53
58	U	101	EHZ	O3-C12	-2.41	1.18	1.23
53	X	1701	CDL	OB8-CB7	2.40	1.40	1.33
48	M	604	PC1	O31-C3	-2.39	1.39	1.45
46	J	401	3PE	O31-C31	2.38	1.40	1.33
46	Y	401	3PE	O31-C31	2.38	1.40	1.33
58	T	101	EHZ	O3-C12	-2.37	1.18	1.23
53	L	704	CDL	OA6-CA4	-2.37	1.40	1.46
46	A	302	3PE	O31-C31	2.37	1.40	1.33
46	O	1201	3PE	O31-C31	2.36	1.40	1.33
46	M	601	3PE	O21-C2	-2.35	1.40	1.46
53	q	201	CDL	OA8-CA6	-2.35	1.39	1.45
46	M	603	3PE	O31-C31	2.34	1.40	1.33
46	b	901	3PE	O31-C3	-2.32	1.39	1.45
53	L	704	CDL	OB8-CB7	2.32	1.40	1.33
54	O	1202	GTP	PG-O2G	-2.31	1.45	1.54
53	K	401	CDL	OA8-CA6	-2.30	1.39	1.45
48	B	203	PC1	O31-C3	-2.29	1.39	1.45
53	L	704	CDL	OB8-CB6	-2.29	1.39	1.45
53	h	1001	CDL	OA8-CA7	2.28	1.40	1.33
54	O	1202	GTP	PG-O3G	-2.28	1.46	1.54
53	K	401	CDL	OA8-CA7	2.28	1.40	1.33
56	P	501	NDP	O5D-C5D	-2.26	1.36	1.44
53	d	201	CDL	OA8-CA7	2.25	1.39	1.33
53	d	201	CDL	OA8-CA6	-2.25	1.40	1.45
48	M	604	PC1	O31-C31	2.25	1.39	1.33
48	B	203	PC1	O21-C21	2.24	1.40	1.34
53	q	201	CDL	OB8-CB6	-2.24	1.40	1.45
46	M	603	3PE	O31-C3	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	O	1201	3PE	O31-C3	-2.22	1.40	1.45
48	B	203	PC1	O31-C31	2.22	1.39	1.33
45	J	402	LMT	O5B-C5B	2.21	1.49	1.44
46	Y	401	3PE	O31-C3	-2.21	1.40	1.45
53	L	704	CDL	OA6-CA5	2.19	1.40	1.34
46	M	601	3PE	O31-C31	2.19	1.39	1.33
45	M	606	LMT	O5'-C5'	2.19	1.49	1.44
53	h	1001	CDL	OA8-CA6	-2.17	1.40	1.45
46	N	502	3PE	O31-C31	2.17	1.39	1.33
46	I	201	3PE	O21-C21	2.17	1.40	1.34
46	L	703	3PE	O31-C31	2.16	1.39	1.33
46	H	601	3PE	O31-C31	2.16	1.39	1.33
46	H	601	3PE	O31-C3	-2.16	1.40	1.45
46	M	601	3PE	O31-C3	-2.15	1.40	1.45
48	M	604	PC1	O21-C21	2.15	1.40	1.34
53	K	401	CDL	OB6-CB5	2.15	1.40	1.34
45	L	702	LMT	O5B-C5B	2.14	1.49	1.44
53	d	201	CDL	OB6-CB5	2.14	1.40	1.34
58	U	101	EHZ	C9-S1	2.14	1.81	1.76
46	b	901	3PE	O31-C31	2.14	1.39	1.33
53	d	201	CDL	OA6-CA5	2.13	1.40	1.34
53	K	401	CDL	OB8-CB6	-2.13	1.40	1.45
45	N	501	LMT	O5B-C5B	2.12	1.49	1.44
53	h	1001	CDL	OB8-CB7	2.12	1.39	1.33
46	A	302	3PE	O31-C3	-2.12	1.40	1.45
46	A	302	3PE	O21-C21	2.11	1.40	1.34
50	F	501	FMN	C10-N1	2.11	1.37	1.33
46	N	502	3PE	O21-C21	2.11	1.40	1.34
53	q	201	CDL	OA8-CA7	2.11	1.39	1.33
45	A	301	LMT	O5'-C5'	2.11	1.49	1.44
53	L	704	CDL	OB6-CB5	2.11	1.40	1.34
53	K	401	CDL	OA6-CA5	2.10	1.40	1.34
46	J	401	3PE	O31-C3	-2.10	1.40	1.45
46	M	601	3PE	O21-C21	2.09	1.40	1.34
46	b	901	3PE	O21-C21	2.09	1.40	1.34
45	M	606	LMT	O1B-C4'	2.09	1.49	1.43
53	L	704	CDL	OA8-CA6	-2.07	1.40	1.45
58	T	101	EHZ	C9-S1	2.06	1.81	1.76
53	q	201	CDL	OB6-CB5	2.06	1.40	1.34
45	A	301	LMT	O1B-C4'	2.05	1.49	1.43
46	J	401	3PE	O21-C21	2.05	1.40	1.34
45	M	606	LMT	O5B-C5B	2.05	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Y	401	3PE	O21-C21	2.05	1.40	1.34
56	P	501	NDP	O2D-C2D	-2.05	1.38	1.43
45	M	602	LMT	O5B-C5B	2.04	1.49	1.44
45	M	605	LMT	O5B-C5B	2.04	1.49	1.44
53	d	201	CDL	OB8-CB6	-2.04	1.40	1.45
46	I	201	3PE	O31-C31	2.04	1.39	1.33
53	X	1701	CDL	OB6-CB5	2.03	1.40	1.34
45	L	705	LMT	O5B-C5B	2.03	1.49	1.44
46	O	1201	3PE	O21-C21	2.03	1.40	1.34
45	l	201	LMT	O5B-C5B	2.03	1.49	1.44
53	X	1701	CDL	OB8-CB6	-2.03	1.40	1.45
50	F	501	FMN	C4A-C10	-2.02	1.38	1.44
58	U	101	EHZ	O6-C20	-2.01	1.39	1.44
46	M	603	3PE	O21-C21	2.01	1.40	1.34
53	X	1701	CDL	OA6-CA5	2.00	1.40	1.34

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	H	602	I49	C14-N02-C15	-9.16	109.95	125.21
56	P	501	NDP	PN-O3-PA	-6.72	109.75	132.83
58	U	101	EHZ	C8-C9-S1	5.97	121.01	113.63
58	T	101	EHZ	C8-C9-S1	5.39	120.30	113.63
52	N	503	I49	N01-C14-N03	4.83	129.32	120.26
53	L	704	CDL	OA6-CA5-C11	4.50	121.21	111.50
53	h	1001	CDL	OB6-CB5-C51	4.45	121.10	111.50
53	d	201	CDL	OA6-CA5-C11	4.16	120.47	111.50
48	B	203	PC1	O21-C21-C22	4.15	120.44	111.50
53	X	1701	CDL	OB6-CB5-C51	4.12	120.39	111.50
46	A	302	3PE	O21-C21-C22	4.10	120.33	111.50
46	M	603	3PE	O21-C21-C22	4.04	120.20	111.50
46	M	601	3PE	O21-C21-C22	4.04	120.20	111.50
46	Y	401	3PE	O21-C21-C22	4.03	120.19	111.50
46	N	502	3PE	O21-C21-C22	4.02	120.17	111.50
52	H	602	I49	N01-C14-N03	4.01	127.78	120.26
53	X	1701	CDL	OA6-CA5-C11	4.00	120.13	111.50
46	H	601	3PE	O21-C21-O22	-3.94	120.55	125.57
46	O	1201	3PE	O21-C21-C22	3.94	119.98	111.50
48	M	604	PC1	O21-C21-C22	3.90	119.91	111.50
53	h	1001	CDL	OA6-CA5-C11	3.81	119.72	111.50
46	J	401	3PE	O21-C21-C22	3.76	119.60	111.50
53	q	201	CDL	OB6-CB5-C51	3.72	119.52	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	L	703	3PE	O21-C21-C22	3.70	119.48	111.50
45	M	602	LMT	C1'-C2'-C3'	3.68	117.66	110.00
53	K	401	CDL	OA6-CA5-C11	3.60	119.26	111.50
46	I	201	3PE	O21-C21-C22	3.60	119.25	111.50
46	L	701	3PE	O21-C21-C22	3.57	119.20	111.50
46	b	901	3PE	O21-C21-C22	3.56	119.17	111.50
53	K	401	CDL	OB6-CB5-C51	3.53	119.11	111.50
53	L	704	CDL	OB6-CB5-C51	3.49	119.03	111.50
53	d	201	CDL	OB6-CB5-C51	3.48	120.49	110.80
53	q	201	CDL	OA6-CA5-C11	3.45	118.94	111.50
56	P	501	NDP	O2B-P2B-O1X	-3.43	96.17	109.39
50	F	501	FMN	C4-N3-C2	-3.35	119.46	125.64
45	L	705	LMT	C1B-O1B-C4'	-3.30	109.79	117.96
45	h	1002	LMT	O5'-C5'-C4'	3.29	116.69	109.75
54	O	1202	GTP	C3'-C2'-C1'	3.27	105.90	100.98
54	O	1202	GTP	C5-C6-N1	3.20	119.61	113.95
45	M	606	LMT	C1'-O5'-C5'	3.16	119.89	113.69
54	O	1202	GTP	C2-N1-C6	-3.13	119.33	125.10
46	J	401	3PE	O31-C31-C32	3.11	121.67	111.91
50	F	501	FMN	C4A-C10-N10	2.98	120.83	116.48
54	O	1202	GTP	O3G-PG-O3B	2.97	114.59	104.64
45	L	702	LMT	O5B-C5B-C4B	2.93	115.02	109.69
53	h	1001	CDL	OA8-CA7-C31	2.91	121.05	111.91
46	M	603	3PE	O31-C31-C32	2.91	121.05	111.91
46	Y	401	3PE	O31-C31-C32	2.86	120.89	111.91
50	F	501	FMN	C4A-C4-N3	2.85	120.43	113.19
54	O	1202	GTP	PA-O3A-PB	-2.83	123.11	132.83
46	H	601	3PE	O31-C31-C32	2.82	120.76	111.91
56	P	501	NDP	PA-O5B-C5B	-2.81	105.23	121.68
45	L	702	LMT	C3B-C4B-C5B	2.79	115.21	110.24
53	q	201	CDL	OA8-CA7-C31	2.76	120.58	111.91
54	O	1202	GTP	O2G-PG-O3B	2.75	113.86	104.64
45	M	606	LMT	O1B-C4'-C5'	2.75	116.98	109.45
56	P	501	NDP	PN-O5D-C5D	-2.75	105.58	121.68
53	X	1701	CDL	OB8-CB7-C71	2.74	120.52	111.91
46	L	703	3PE	O31-C31-C32	2.74	120.51	111.91
46	O	1201	3PE	O31-C31-C32	2.73	120.47	111.91
46	M	601	3PE	O31-C31-C32	2.72	120.46	111.91
46	A	302	3PE	O31-C31-C32	2.72	120.45	111.91
52	H	602	I49	N05-C15-N04	-2.69	111.99	120.26
53	d	201	CDL	OA8-CA7-C31	2.69	120.34	111.91
52	N	503	I49	N05-C15-N04	-2.67	112.03	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	H	602	I49	C08-N01-C14	-2.67	118.63	123.50
45	M	602	LMT	C1B-O5B-C5B	-2.66	108.46	113.69
52	N	503	I49	C14-N02-C15	-2.64	120.81	125.21
46	b	901	3PE	O31-C31-C32	2.63	120.17	111.91
53	L	704	CDL	OA8-CA7-C31	2.59	120.03	111.91
53	d	201	CDL	OB8-CB7-C71	2.58	119.99	111.91
50	F	501	FMN	O4-C4-C4A	-2.57	119.78	126.60
48	B	203	PC1	O31-C31-C32	2.57	119.97	111.91
53	h	1001	CDL	OB8-CB7-C71	2.55	119.92	111.91
53	L	704	CDL	OB8-CB7-C71	2.54	119.89	111.91
58	T	101	EHZ	O2-C9-S1	-2.54	119.31	122.61
48	M	604	PC1	O31-C31-C32	2.52	119.80	111.91
56	P	501	NDP	O3X-P2B-O2X	2.51	117.25	107.64
54	O	1202	GTP	PB-O3B-PG	-2.51	124.23	132.83
53	K	401	CDL	OB8-CB7-C71	2.49	119.73	111.91
45	M	606	LMT	O5’-C1’-C2’	2.49	115.62	110.35
52	H	602	I49	N05-C15-N02	2.47	127.60	117.44
52	N	503	I49	N05-C15-N02	2.47	127.59	117.44
56	P	501	NDP	O5D-PN-O1N	-2.47	99.42	109.07
54	O	1202	GTP	C2’-C3’-C4’	2.43	107.37	102.64
46	N	502	3PE	O31-C31-C32	2.42	119.51	111.91
45	M	602	LMT	C2’-C3’-C4’	2.42	115.21	109.68
53	K	401	CDL	OA8-CA7-C31	2.42	119.50	111.91
46	I	201	3PE	O31-C31-C32	2.41	119.46	111.91
54	O	1202	GTP	O2A-PA-O1A	-2.39	100.44	112.24
58	U	101	EHZ	C16-C15-N2	2.38	121.32	116.58
50	F	501	FMN	C10-C4A-N5	-2.37	119.83	124.86
58	T	101	EHZ	C13-C12-N1	2.37	120.41	116.42
53	q	201	CDL	OB8-CB7-C71	2.36	119.32	111.91
45	L	702	LMT	C6B-C5B-C4B	-2.32	107.56	113.00
56	P	501	NDP	O4B-C4B-C3B	2.32	109.70	105.11
54	O	1202	GTP	O2B-PB-O1B	-2.31	100.80	112.24
52	H	602	I49	C12-C13-I02	-2.29	119.30	121.72
50	F	501	FMN	C4A-C10-N1	-2.28	119.43	124.73
45	N	501	LMT	O1B-C4’-C3’	2.28	113.35	107.28
46	L	701	3PE	O31-C31-C32	2.27	119.02	111.91
45	L	702	LMT	C1B-O1B-C4’	-2.26	112.36	117.96
45	h	1002	LMT	C1B-O1B-C4’	-2.26	112.36	117.96
45	L	705	LMT	C2’-C3’-C4’	2.24	114.79	109.68
56	P	501	NDP	C2A-N1A-C6A	-2.24	114.93	118.75
56	P	501	NDP	O2N-PN-O1N	2.23	123.25	112.24
52	N	503	I49	C09-C07-C10	2.22	121.65	118.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	B	202	LMT	O1'-C1'-C2'	2.21	111.75	108.30
45	f	1901	LMT	C1'-C2'-C3'	2.19	114.56	110.00
45	M	606	LMT	C3B-C4B-C5B	2.18	114.13	110.24
45	h	1002	LMT	C2'-C3'-C4'	2.16	114.61	109.68
58	U	101	EHZ	C13-C12-N1	2.14	120.02	116.42
45	L	705	LMT	C1'-C2'-C3'	2.14	114.44	110.00
52	H	602	I49	C09-C07-C10	2.13	121.53	118.54
58	U	101	EHZ	O2-C9-S1	-2.12	119.87	122.61
56	P	501	NDP	C5B-C4B-C3B	-2.10	107.31	115.18
45	h	1002	LMT	C3'-C4'-C5'	2.07	115.67	110.93
45	f	1901	LMT	C1B-O1B-C4'	-2.06	112.87	117.96
45	A	301	LMT	O1B-C4'-C3'	2.05	112.73	107.28
45	L	706	LMT	C1B-O5B-C5B	-2.05	109.67	113.69
53	X	1701	CDL	CA4-OA6-CA5	-2.03	112.78	117.79
54	O	1202	GTP	O6-C6-C5	-2.02	120.42	124.37
56	P	501	NDP	O7N-C7N-N7N	-2.02	118.16	122.88
45	M	605	LMT	C2'-C3'-C4'	2.01	114.28	109.68
45	f	1901	LMT	C2'-C3'-C4'	2.00	114.26	109.68

There are no chirality outliers.

All (623) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	301	LMT	C2'-C1'-O1'-C1
45	A	301	LMT	O5'-C1'-O1'-C1
45	J	402	LMT	C2-C1-O1'-C1'
45	L	705	LMT	O5'-C1'-O1'-C1
45	L	706	LMT	C2-C1-O1'-C1'
45	f	1901	LMT	C2'-C1'-O1'-C1
45	f	1901	LMT	O5'-C1'-O1'-C1
46	A	302	3PE	O13-C11-C12-N
46	A	302	3PE	O22-C21-O21-C2
46	A	302	3PE	C22-C21-O21-C2
46	H	601	3PE	C1-O11-P-O14
46	H	601	3PE	C11-O13-P-O11
46	H	601	3PE	C11-O13-P-O12
46	H	601	3PE	O13-C11-C12-N
46	H	601	3PE	O22-C21-O21-C2
46	I	201	3PE	C11-O13-P-O14
46	I	201	3PE	O13-C11-C12-N
46	J	401	3PE	C1-O11-P-O14
46	J	401	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
46	J	401	3PE	O13-C11-C12-N
46	L	701	3PE	O13-C11-C12-N
46	L	703	3PE	O13-C11-C12-N
46	M	601	3PE	C1-O11-P-O14
46	M	601	3PE	O13-C11-C12-N
46	M	603	3PE	C11-O13-P-O12
46	N	502	3PE	C1-O11-P-O14
46	N	502	3PE	C11-O13-P-O14
46	N	502	3PE	O13-C11-C12-N
46	O	1201	3PE	C1-O11-P-O12
46	O	1201	3PE	C1-O11-P-O13
46	O	1201	3PE	C1-O11-P-O14
46	O	1201	3PE	C22-C21-O21-C2
46	Y	401	3PE	C22-C21-O21-C2
46	b	901	3PE	C11-O13-P-O12
46	b	901	3PE	O21-C2-C3-O31
48	B	203	PC1	C11-O13-P-O12
48	B	203	PC1	C11-O13-P-O14
48	M	604	PC1	O21-C2-C3-O31
52	H	602	I49	N05-C15-N02-C14
52	N	503	I49	C07-C06-C08-N01
52	N	503	I49	N01-C14-N02-C15
52	N	503	I49	N03-C14-N02-C15
53	K	401	CDL	O1-C1-CB2-OB2
53	K	401	CDL	CB3-OB5-PB2-OB2
53	K	401	CDL	CB3-OB5-PB2-OB3
53	L	704	CDL	OA7-CA5-OA6-CA4
53	L	704	CDL	C11-CA5-OA6-CA4
53	X	1701	CDL	CA2-OA2-PA1-OA4
53	X	1701	CDL	CA3-OA5-PA1-OA3
53	X	1701	CDL	CA3-OA5-PA1-OA4
53	X	1701	CDL	OA9-CA7-OA8-CA6
53	X	1701	CDL	CB2-OB2-PB2-OB3
53	X	1701	CDL	OB6-CB4-CB6-OB8
53	X	1701	CDL	OB9-CB7-OB8-CB6
53	d	201	CDL	CA2-OA2-PA1-OA3
53	d	201	CDL	CB3-OB5-PB2-OB3
53	d	201	CDL	CB3-OB5-PB2-OB4
53	d	201	CDL	OB7-CB5-OB6-CB4
53	h	1001	CDL	CA2-C1-CB2-OB2
53	h	1001	CDL	CB3-OB5-PB2-OB3
53	h	1001	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
53	h	1001	CDL	C51-CB5-OB6-CB4
53	q	201	CDL	CA2-OA2-PA1-OA4
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CB3-OB5-PB2-OB3
54	O	1202	GTP	C5'-O5'-PA-O3A
56	P	501	NDP	C2B-O2B-P2B-O3X
58	T	101	EHZ	O1-C7-C8-C9
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-O5
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
45	M	606	LMT	C5'-C4'-O1B-C1B
46	J	401	3PE	O32-C31-O31-C3
45	M	605	LMT	O5B-C1B-O1B-C4'
46	J	401	3PE	C32-C31-O31-C3
46	L	703	3PE	O32-C31-O31-C3
46	O	1201	3PE	O32-C31-O31-C3
46	Y	401	3PE	O32-C31-O31-C3
53	L	704	CDL	OA9-CA7-OA8-CA6
46	O	1201	3PE	O22-C21-O21-C2
45	A	301	LMT	C3'-C4'-O1B-C1B
46	M	603	3PE	C32-C31-O31-C3
46	O	1201	3PE	C32-C31-O31-C3
46	Y	401	3PE	C32-C31-O31-C3
53	L	704	CDL	C31-CA7-OA8-CA6
53	X	1701	CDL	C71-CB7-OB8-CB6
53	d	201	CDL	C51-CB5-OB6-CB4
45	J	402	LMT	O5B-C1B-O1B-C4'
45	N	501	LMT	C3'-C4'-O1B-C1B
46	L	703	3PE	C32-C31-O31-C3
53	d	201	CDL	C71-CB7-OB8-CB6
45	A	301	LMT	O5B-C5B-C6B-O6B
46	Y	401	3PE	O22-C21-O21-C2
45	h	1002	LMT	C2-C3-C4-C5
45	M	606	LMT	O5B-C1B-O1B-C4'
45	J	402	LMT	C2B-C1B-O1B-C4'
45	M	606	LMT	O5B-C5B-C6B-O6B
45	N	501	LMT	O5'-C5'-C6'-O6'
45	f	1901	LMT	O5'-C5'-C6'-O6'
45	l	201	LMT	C4'-C5'-C6'-O6'
53	h	1001	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
48	B	203	PC1	C32-C31-O31-C3
46	M	603	3PE	O32-C31-O31-C3
45	L	706	LMT	O5'-C5'-C6'-O6'
53	q	201	CDL	C11-CA5-OA6-CA4
45	M	606	LMT	C2B-C1B-O1B-C4'
45	M	605	LMT	O5B-C5B-C6B-O6B
45	A	301	LMT	C4B-C5B-C6B-O6B
45	N	501	LMT	C4'-C5'-C6'-O6'
45	B	202	LMT	C3'-C4'-O1B-C1B
45	J	402	LMT	O5'-C5'-C6'-O6'
45	M	606	LMT	C4B-C5B-C6B-O6B
45	f	1901	LMT	C4'-C5'-C6'-O6'
48	M	604	PC1	C2-C1-O11-P
45	A	301	LMT	O5'-C5'-C6'-O6'
45	L	706	LMT	O5B-C5B-C6B-O6B
53	d	201	CDL	OB9-CB7-OB8-CB6
45	N	501	LMT	O5'-C1'-O1'-C1
45	M	602	LMT	O5B-C5B-C6B-O6B
45	L	706	LMT	C4'-C5'-C6'-O6'
48	B	203	PC1	O32-C31-O31-C3
46	L	701	3PE	C22-C21-O21-C2
53	K	401	CDL	CA2-C1-CB2-OB2
46	N	502	3PE	C32-C31-O31-C3
48	M	604	PC1	C32-C31-O31-C3
53	h	1001	CDL	C31-CA7-OA8-CA6
46	L	701	3PE	C31-C32-C33-C34
46	A	302	3PE	O11-C1-C2-O21
45	L	706	LMT	C2'-C1'-O1'-C1
45	l	201	LMT	O5'-C5'-C6'-O6'
45	A	301	LMT	C4'-C5'-C6'-O6'
45	L	706	LMT	C4B-C5B-C6B-O6B
45	M	605	LMT	C4B-C5B-C6B-O6B
46	M	601	3PE	C21-C22-C23-C24
45	f	1901	LMT	O5B-C1B-O1B-C4'
48	M	604	PC1	O32-C31-O31-C3
46	M	603	3PE	C21-C22-C23-C24
53	K	401	CDL	CA5-C11-C12-C13
45	L	705	LMT	O5'-C5'-C6'-O6'
46	N	502	3PE	O32-C31-O31-C3
46	A	302	3PE	C21-C22-C23-C24
46	J	401	3PE	C31-C32-C33-C34
46	O	1201	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
46	Y	401	3PE	C31-C32-C33-C34
53	h	1001	CDL	CB5-C51-C52-C53
56	P	501	NDP	O4D-C4D-C5D-O5D
53	q	201	CDL	C71-CB7-OB8-CB6
53	q	201	CDL	OA7-CA5-OA6-CA4
45	L	702	LMT	O1'-C1-C2-C3
53	L	704	CDL	CB5-C51-C52-C53
45	h	1002	LMT	C4B-C5B-C6B-O6B
53	L	704	CDL	C83-C84-C85-C86
53	h	1001	CDL	OA9-CA7-OA8-CA6
45	J	402	LMT	C4'-C5'-C6'-O6'
45	f	1901	LMT	O5B-C5B-C6B-O6B
53	X	1701	CDL	O1-C1-CA2-OA2
46	L	701	3PE	O22-C21-O21-C2
53	d	201	CDL	C31-CA7-OA8-CA6
45	L	705	LMT	C4'-C5'-C6'-O6'
46	L	703	3PE	C22-C21-O21-C2
59	o	201	MYR	C6-C7-C8-C9
46	J	401	3PE	C11-O13-P-O11
46	M	603	3PE	C11-O13-P-O11
46	N	502	3PE	C1-O11-P-O13
46	N	502	3PE	C11-O13-P-O11
46	b	901	3PE	C11-O13-P-O11
48	B	203	PC1	C11-O13-P-O11
53	X	1701	CDL	CA2-OA2-PA1-OA5
53	X	1701	CDL	CA3-OA5-PA1-OA2
53	d	201	CDL	CB3-OB5-PB2-OB2
53	h	1001	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	CB3-OB5-PB2-OB2
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CB3-OB5-PB2-OB2
53	h	1001	CDL	C71-CB7-OB8-CB6
53	q	201	CDL	C31-CA7-OA8-CA6
53	X	1701	CDL	CB2-C1-CA2-OA2
46	L	703	3PE	O22-C21-O21-C2
53	q	201	CDL	OB9-CB7-OB8-CB6
45	N	501	LMT	C4B-C5B-C6B-O6B
46	M	603	3PE	C3A-C3B-C3C-C3D
46	b	901	3PE	C28-C29-C2A-C2B
53	L	704	CDL	C37-C38-C39-C40
53	X	1701	CDL	C11-CA5-OA6-CA4
53	d	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
45	J	402	LMT	C4-C5-C6-C7
46	I	201	3PE	C2C-C2D-C2E-C2F
53	L	704	CDL	C79-C80-C81-C82
53	X	1701	CDL	C15-C16-C17-C18
53	h	1001	CDL	C12-C13-C14-C15
53	q	201	CDL	C51-C52-C53-C54
53	q	201	CDL	C56-C57-C58-C59
46	I	201	3PE	C3A-C3B-C3C-C3D
46	L	701	3PE	C2E-C2F-C2G-C2H
53	L	704	CDL	C53-C54-C55-C56
53	X	1701	CDL	C11-C12-C13-C14
53	X	1701	CDL	C55-C56-C57-C58
53	X	1701	CDL	OA7-CA5-OA6-CA4
53	d	201	CDL	OA7-CA5-OA6-CA4
53	d	201	CDL	OA9-CA7-OA8-CA6
45	B	202	LMT	C3-C4-C5-C6
46	M	601	3PE	C28-C29-C2A-C2B
46	O	1201	3PE	C3B-C3C-C3D-C3E
58	U	101	EHZ	C1-C2-C3-C4
53	d	201	CDL	O1-C1-CB2-OB2
46	b	901	3PE	C24-C25-C26-C27
46	Y	401	3PE	C37-C38-C39-C3A
46	b	901	3PE	C27-C28-C29-C2A
53	K	401	CDL	C38-C39-C40-C41
59	o	201	MYR	C10-C11-C12-C13
53	L	704	CDL	C74-C75-C76-C77
53	q	201	CDL	C37-C38-C39-C40
53	X	1701	CDL	CB5-C51-C52-C53
45	L	706	LMT	C5-C6-C7-C8
46	I	201	3PE	C33-C34-C35-C36
53	K	401	CDL	C40-C41-C42-C43
59	o	201	MYR	C7-C8-C9-C10
53	K	401	CDL	OA7-CA5-OA6-CA4
53	K	401	CDL	C11-CA5-OA6-CA4
53	d	201	CDL	C33-C34-C35-C36
46	I	201	3PE	C21-C22-C23-C24
46	J	401	3PE	C32-C33-C34-C35
46	L	703	3PE	C3C-C3D-C3E-C3F
53	L	704	CDL	C63-C64-C65-C66
59	o	201	MYR	C11-C10-C9-C8
53	h	1001	CDL	C72-C73-C74-C75
46	N	502	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
53	K	401	CDL	C12-C13-C14-C15
53	h	1001	CDL	C32-C33-C34-C35
46	O	1201	3PE	C21-C22-C23-C24
53	q	201	CDL	OA9-CA7-OA8-CA6
53	L	704	CDL	C38-C39-C40-C41
45	f	1901	LMT	C3-C4-C5-C6
46	N	502	3PE	C22-C23-C24-C25
53	L	704	CDL	C60-C61-C62-C63
46	M	603	3PE	C2E-C2F-C2G-C2H
53	L	704	CDL	C43-C44-C45-C46
45	f	1901	LMT	C1-C2-C3-C4
46	L	703	3PE	C25-C26-C27-C28
46	M	603	3PE	C3D-C3E-C3F-C3G
53	q	201	CDL	C58-C59-C60-C61
53	h	1001	CDL	OB9-CB7-OB8-CB6
46	M	603	3PE	C39-C3A-C3B-C3C
46	M	603	3PE	C27-C28-C29-C2A
46	b	901	3PE	C35-C36-C37-C38
48	M	604	PC1	C27-C28-C29-C2A
46	L	703	3PE	C31-C32-C33-C34
53	d	201	CDL	CA2-C1-CB2-OB2
58	U	101	EHZ	C3-C4-C5-C6
46	L	701	3PE	C29-C2A-C2B-C2C
45	N	501	LMT	O5B-C5B-C6B-O6B
53	L	704	CDL	C58-C59-C60-C61
45	N	501	LMT	C1-C2-C3-C4
46	I	201	3PE	C25-C26-C27-C28
48	M	604	PC1	C2B-C2C-C2D-C2E
46	O	1201	3PE	C37-C38-C39-C3A
48	M	604	PC1	C2C-C2D-C2E-C2F
45	M	605	LMT	C2B-C1B-O1B-C4’
58	T	101	EHZ	C5-C6-C7-C8
53	L	704	CDL	C17-C18-C19-C20
58	U	101	EHZ	C1-C21-C22-C23
52	H	602	I49	N04-C15-N02-C14
53	L	704	CDL	CB7-C71-C72-C73
53	K	401	CDL	C53-C54-C55-C56
46	N	502	3PE	C27-C28-C29-C2A
45	L	706	LMT	O5’-C1’-O1’-C1
46	b	901	3PE	C23-C24-C25-C26
53	q	201	CDL	C13-C14-C15-C16
59	o	201	MYR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
53	q	201	CDL	OB5-CB3-CB4-OB6
53	h	1001	CDL	C16-C17-C18-C19
45	l	201	LMT	O5B-C1B-O1B-C4'
46	L	701	3PE	C32-C31-O31-C3
53	X	1701	CDL	C51-C52-C53-C54
46	N	502	3PE	C24-C25-C26-C27
45	h	1002	LMT	O5B-C5B-C6B-O6B
53	d	201	CDL	CA2-OA2-PA1-OA5
53	q	201	CDL	CA2-OA2-PA1-OA5
59	o	201	MYR	C9-C10-C11-C12
46	L	703	3PE	C37-C38-C39-C3A
53	K	401	CDL	C33-C34-C35-C36
46	A	302	3PE	O11-C1-C2-C3
46	Y	401	3PE	O11-C1-C2-C3
48	B	203	PC1	C33-C34-C35-C36
53	X	1701	CDL	C17-C18-C19-C20
46	L	701	3PE	C36-C37-C38-C39
46	A	302	3PE	C33-C34-C35-C36
53	q	201	CDL	C52-C53-C54-C55
53	L	704	CDL	C20-C21-C22-C23
46	I	201	3PE	C2B-C2C-C2D-C2E
46	N	502	3PE	C23-C24-C25-C26
46	L	701	3PE	C34-C35-C36-C37
53	X	1701	CDL	C51-CB5-OB6-CB4
53	X	1701	CDL	C74-C75-C76-C77
46	O	1201	3PE	C1-C2-C3-O31
46	Y	401	3PE	C1-C2-C3-O31
46	b	901	3PE	C1-C2-C3-O31
48	B	203	PC1	C1-C2-C3-O31
48	M	604	PC1	C32-C33-C34-C35
45	M	605	LMT	O5'-C1'-O1'-C1
58	T	101	EHZ	O4-C15-C16-O5
53	L	704	CDL	C16-C17-C18-C19
46	N	502	3PE	C22-C21-O21-C2
58	T	101	EHZ	C5-C6-C7-O1
53	L	704	CDL	C42-C43-C44-C45
45	L	705	LMT	O5B-C5B-C6B-O6B
46	M	603	3PE	C33-C34-C35-C36
46	Y	401	3PE	C2-C1-O11-P
46	L	703	3PE	C35-C36-C37-C38
53	h	1001	CDL	OB6-CB4-CB6-OB8
46	I	201	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	O32-C31-O31-C3
46	Y	401	3PE	C23-C24-C25-C26
46	L	703	3PE	C29-C2A-C2B-C2C
53	d	201	CDL	CA5-C11-C12-C13
53	q	201	CDL	C60-C61-C62-C63
46	b	901	3PE	C32-C31-O31-C3
53	L	704	CDL	C24-C25-C26-C27
53	X	1701	CDL	C58-C59-C60-C61
45	A	301	LMT	C1-C2-C3-C4
53	d	201	CDL	C76-C77-C78-C79
53	d	201	CDL	C31-C32-C33-C34
46	L	703	3PE	O11-C1-C2-C3
46	M	601	3PE	O11-C1-C2-C3
53	K	401	CDL	OB5-CB3-CB4-CB6
53	d	201	CDL	OA5-CA3-CA4-CA6
53	d	201	CDL	CA7-C31-C32-C33
45	M	602	LMT	C4B-C5B-C6B-O6B
58	T	101	EHZ	O4-C15-C16-C17
45	l	201	LMT	C4-C5-C6-C7
46	L	701	3PE	C37-C38-C39-C3A
45	f	1901	LMT	C3'-C4'-O1B-C1B
46	I	201	3PE	C27-C28-C29-C2A
53	K	401	CDL	C31-CA7-OA8-CA6
46	M	603	3PE	C31-C32-C33-C34
45	B	202	LMT	C5'-C4'-O1B-C1B
53	K	401	CDL	CB4-CB3-OB5-PB2
45	M	606	LMT	O5'-C5'-C6'-O6'
45	M	602	LMT	C2-C1-O1'-C1'
53	L	704	CDL	C72-C73-C74-C75
46	L	701	3PE	C1-C2-C3-O31
46	M	601	3PE	C1-C2-C3-O31
48	M	604	PC1	C1-C2-C3-O31
53	h	1001	CDL	CB3-CB4-CB6-OB8
53	h	1001	CDL	C15-C16-C17-C18
58	T	101	EHZ	N2-C15-C16-C17
46	M	601	3PE	C1-O11-P-O13
45	f	1901	LMT	C5'-C4'-O1B-C1B
53	d	201	CDL	C38-C39-C40-C41
53	d	201	CDL	OB5-CB3-CB4-OB6
53	d	201	CDL	C77-C78-C79-C80
46	I	201	3PE	O32-C31-O31-C3
48	B	203	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
53	X	1701	CDL	C76-C77-C78-C79
58	U	101	EHZ	C2-C3-C4-C5
46	L	701	3PE	C22-C23-C24-C25
46	J	401	3PE	O21-C2-C3-O31
46	L	701	3PE	O21-C2-C3-O31
46	M	601	3PE	O21-C2-C3-O31
46	Y	401	3PE	O21-C2-C3-O31
45	M	605	LMT	C2-C3-C4-C5
46	A	302	3PE	C23-C24-C25-C26
46	N	502	3PE	O22-C21-O21-C2
53	X	1701	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	CA4-CA3-OA5-PA1
48	M	604	PC1	C29-C2A-C2B-C2C
45	A	301	LMT	C2-C3-C4-C5
46	Y	401	3PE	C3B-C3C-C3D-C3E
53	K	401	CDL	C36-C37-C38-C39
46	M	603	3PE	C36-C37-C38-C39
53	L	704	CDL	C13-C14-C15-C16
58	U	101	EHZ	C22-C23-C24-C25
46	Y	401	3PE	C34-C35-C36-C37
46	M	603	3PE	C35-C36-C37-C38
46	b	901	3PE	O32-C31-O31-C3
48	M	604	PC1	C23-C24-C25-C26
46	M	603	3PE	O11-C1-C2-C3
53	X	1701	CDL	C56-C57-C58-C59
46	J	401	3PE	C27-C28-C29-C2A
46	L	703	3PE	C38-C39-C3A-C3B
46	O	1201	3PE	C36-C37-C38-C39
46	M	603	3PE	C22-C21-O21-C2
45	l	201	LMT	C1-C2-C3-C4
56	P	501	NDP	C2B-O2B-P2B-O1X
46	H	601	3PE	C36-C37-C38-C39
45	L	706	LMT	O1'-C1-C2-C3
48	M	604	PC1	C2F-C2G-C2H-C2I
48	M	604	PC1	C2E-C2F-C2G-C2H
53	q	201	CDL	C15-C16-C17-C18
46	L	703	3PE	C39-C3A-C3B-C3C
46	N	502	3PE	C33-C34-C35-C36
45	B	202	LMT	O5'-C1'-O1'-C1
46	H	601	3PE	C33-C34-C35-C36
46	A	302	3PE	C1-C2-C3-O31
46	J	401	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	M	603	3PE	C2-C1-O11-P
52	H	602	I49	N01-C14-N02-C15
53	K	401	CDL	C1-CB2-OB2-PB2
53	h	1001	CDL	CA3-CA4-CA6-OA8
46	L	703	3PE	O11-C1-C2-O21
46	b	901	3PE	O11-C1-C2-O21
53	K	401	CDL	OB5-CB3-CB4-OB6
53	L	704	CDL	OA5-CA3-CA4-OA6
53	X	1701	CDL	OA5-CA3-CA4-OA6
53	d	201	CDL	OA5-CA3-CA4-OA6
52	H	602	I49	C07-C06-C08-N01
46	M	603	3PE	O22-C21-O21-C2
46	N	502	3PE	C32-C33-C34-C35
46	N	502	3PE	C26-C27-C28-C29
53	L	704	CDL	C71-CB7-OB8-CB6
46	O	1201	3PE	C28-C29-C2A-C2B
53	K	401	CDL	OA9-CA7-OA8-CA6
53	L	704	CDL	C11-C12-C13-C14
53	q	201	CDL	C54-C55-C56-C57
46	H	601	3PE	C3A-C3B-C3C-C3D
53	q	201	CDL	C35-C36-C37-C38
45	L	706	LMT	C6-C7-C8-C9
46	J	401	3PE	C1-O11-P-O13
53	d	201	CDL	CB2-OB2-PB2-OB5
56	P	501	NDP	O4D-C1D-N1N-C6N
53	q	201	CDL	CA5-C11-C12-C13
45	M	606	LMT	C4'-C5'-C6'-O6'
45	N	501	LMT	C5'-C4'-O1B-C1B
53	X	1701	CDL	C19-C20-C21-C22
46	H	601	3PE	C11-O13-P-O14
46	J	401	3PE	C11-O13-P-O12
46	J	401	3PE	C11-O13-P-O14
46	M	601	3PE	C1-O11-P-O12
46	N	502	3PE	C11-O13-P-O12
46	b	901	3PE	C11-O13-P-O14
48	M	604	PC1	C11-O13-P-O12
53	X	1701	CDL	CA2-OA2-PA1-OA3
53	d	201	CDL	CB2-OB2-PB2-OB3
53	h	1001	CDL	CA2-OA2-PA1-OA4
53	h	1001	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CA2-OA2-PA1-OA3
54	O	1202	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
54	O	1202	GTP	C5'-O5'-PA-O2A
58	T	101	EHZ	C6-C7-C8-C9
53	L	704	CDL	OA5-CA3-CA4-CA6
53	d	201	CDL	OB5-CB3-CB4-CB6
53	q	201	CDL	OB5-CB3-CB4-CB6
53	L	704	CDL	OB9-CB7-OB8-CB6
46	b	901	3PE	C2A-C2B-C2C-C2D
53	d	201	CDL	C75-C76-C77-C78
46	L	701	3PE	C2A-C2B-C2C-C2D
46	M	601	3PE	C12-C11-O13-P
46	L	701	3PE	C2F-C2G-C2H-C2I
53	q	201	CDL	C16-C17-C18-C19
46	M	601	3PE	O11-C1-C2-O21
46	M	603	3PE	O11-C1-C2-O21
46	Y	401	3PE	O11-C1-C2-O21
56	P	501	NDP	C3D-C4D-C5D-O5D
46	A	302	3PE	C27-C28-C29-C2A
45	f	1901	LMT	C2-C1-O1'-C1'
46	L	701	3PE	C26-C27-C28-C29
53	X	1701	CDL	CB3-CB4-CB6-OB8
46	O	1201	3PE	O21-C2-C3-O31
48	B	203	PC1	O21-C2-C3-O31
53	h	1001	CDL	OA6-CA4-CA6-OA8
46	I	201	3PE	C35-C36-C37-C38
53	h	1001	CDL	C71-C72-C73-C74
45	f	1901	LMT	C4B-C5B-C6B-O6B
46	O	1201	3PE	C3D-C3E-C3F-C3G
53	X	1701	CDL	C52-C53-C54-C55
48	B	203	PC1	C36-C37-C38-C39
46	M	601	3PE	C25-C26-C27-C28
46	M	603	3PE	C2B-C2C-C2D-C2E
46	O	1201	3PE	C23-C24-C25-C26
46	M	601	3PE	C2A-C2B-C2C-C2D
53	K	401	CDL	C71-C72-C73-C74
53	L	704	CDL	C34-C35-C36-C37
46	L	701	3PE	C3A-C3B-C3C-C3D
46	M	601	3PE	C3-C2-O21-C21
53	L	704	CDL	C22-C23-C24-C25
53	L	704	CDL	CA4-CA3-OA5-PA1
46	I	201	3PE	C34-C35-C36-C37
45	L	705	LMT	C2'-C1'-O1'-C1
46	I	201	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
46	Y	401	3PE	C1-O11-P-O13
53	L	704	CDL	CA2-OA2-PA1-OA5
53	q	201	CDL	CB2-OB2-PB2-OB5
53	h	1001	CDL	OA7-CA5-OA6-CA4
53	L	704	CDL	C21-C22-C23-C24
46	O	1201	3PE	C22-C23-C24-C25
46	I	201	3PE	C23-C24-C25-C26
46	I	201	3PE	C31-C32-C33-C34
53	h	1001	CDL	C51-C52-C53-C54
45	l	201	LMT	C3'-C4'-O1B-C1B
46	L	703	3PE	O21-C21-C22-C23
53	K	401	CDL	CB7-C71-C72-C73
46	I	201	3PE	C26-C27-C28-C29
53	q	201	CDL	C72-C73-C74-C75
46	b	901	3PE	O11-C1-C2-C3
46	O	1201	3PE	O13-C11-C12-N
45	J	402	LMT	C3-C4-C5-C6
45	l	201	LMT	O1'-C1-C2-C3
46	L	701	3PE	C2B-C2C-C2D-C2E
46	M	603	3PE	C37-C38-C39-C3A
53	X	1701	CDL	C57-C58-C59-C60
46	H	601	3PE	O11-C1-C2-O21
46	L	701	3PE	C24-C25-C26-C27
46	L	703	3PE	C36-C37-C38-C39
45	L	705	LMT	C3-C4-C5-C6
53	L	704	CDL	C14-C15-C16-C17
45	B	202	LMT	O5B-C5B-C6B-O6B
46	N	502	3PE	C2-C1-O11-P
50	F	501	FMN	C4'-C5'-O5'-P
46	H	601	3PE	C3B-C3C-C3D-C3E
53	L	704	CDL	C32-C33-C34-C35
58	T	101	EHZ	C18-C17-C20-O6
53	K	401	CDL	O1-C1-CA2-OA2
53	X	1701	CDL	C71-C72-C73-C74
53	K	401	CDL	C35-C36-C37-C38
46	L	703	3PE	C3B-C3C-C3D-C3E
46	M	601	3PE	C2E-C2F-C2G-C2H
45	M	605	LMT	O1'-C1-C2-C3
45	l	201	LMT	C5'-C4'-O1B-C1B
46	A	302	3PE	O21-C2-C3-O31
53	L	704	CDL	OB6-CB4-CB6-OB8
45	L	702	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
45	A	301	LMT	C5'-C4'-O1B-C1B
53	h	1001	CDL	C11-CA5-OA6-CA4
53	h	1001	CDL	C24-C25-C26-C27
46	J	401	3PE	C24-C25-C26-C27
45	L	706	LMT	C9-C10-C11-C12
45	M	605	LMT	C9-C10-C11-C12
53	h	1001	CDL	C31-C32-C33-C34
45	N	501	LMT	C4-C5-C6-C7
45	l	201	LMT	C2B-C1B-O1B-C4'
53	X	1701	CDL	OA5-CA3-CA4-CA6
45	M	605	LMT	C5-C6-C7-C8
45	M	602	LMT	C1-C2-C3-C4
46	H	601	3PE	C2-C1-O11-P
53	q	201	CDL	C40-C41-C42-C43
53	d	201	CDL	OB6-CB4-CB6-OB8
53	q	201	CDL	C11-C12-C13-C14
46	J	401	3PE	C23-C24-C25-C26
53	K	401	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	C17-C18-C19-C20
45	L	705	LMT	C4-C5-C6-C7
53	L	704	CDL	C81-C82-C83-C84
45	h	1002	LMT	C2-C1-O1'-C1'
53	L	704	CDL	C36-C37-C38-C39
53	L	704	CDL	C78-C79-C80-C81
53	d	201	CDL	CB3-CB4-CB6-OB8
53	h	1001	CDL	C20-C21-C22-C23
46	M	603	3PE	O21-C21-C22-C23
46	N	502	3PE	O31-C31-C32-C33
46	b	901	3PE	O31-C31-C32-C33
46	J	401	3PE	C38-C39-C3A-C3B
53	L	704	CDL	C55-C56-C57-C58
53	q	201	CDL	C73-C74-C75-C76
48	B	203	PC1	O21-C21-C22-C23
46	M	601	3PE	C22-C23-C24-C25
46	M	603	3PE	C22-C23-C24-C25
46	H	601	3PE	O11-C1-C2-C3
46	J	401	3PE	O11-C1-C2-C3
46	J	401	3PE	O31-C31-C32-C33
46	b	901	3PE	O21-C21-C22-C23
53	X	1701	CDL	OA6-CA4-CA6-OA8
53	q	201	CDL	OB6-CB4-CB6-OB8
46	b	901	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
46	M	601	3PE	C32-C33-C34-C35
53	h	1001	CDL	C22-C23-C24-C25
46	L	701	3PE	C28-C29-C2A-C2B
53	d	201	CDL	C52-C51-CB5-OB6
45	M	606	LMT	C5-C6-C7-C8
54	O	1202	GTP	PA-O3A-PB-O1B
54	O	1202	GTP	PA-O3A-PB-O2B
56	P	501	NDP	PN-O3-PA-O1A
53	K	401	CDL	C14-C15-C16-C17
53	L	704	CDL	C52-C51-CB5-OB6
53	d	201	CDL	C42-C43-C44-C45
46	L	703	3PE	C22-C23-C24-C25
46	A	302	3PE	O31-C31-C32-C33
52	H	602	I49	N03-C14-N02-C15
46	H	601	3PE	C35-C36-C37-C38
46	N	502	3PE	O32-C31-C32-C33
46	b	901	3PE	O32-C31-C32-C33
53	d	201	CDL	C73-C74-C75-C76
53	d	201	CDL	C52-C51-CB5-OB7
46	O	1201	3PE	C2-C1-O11-P
53	h	1001	CDL	C34-C35-C36-C37
46	N	502	3PE	C1-O11-P-O12
46	O	1201	3PE	C11-O13-P-O14
46	Y	401	3PE	C1-O11-P-O14
46	b	901	3PE	C1-O11-P-O14
53	K	401	CDL	CA3-OA5-PA1-OA3
53	L	704	CDL	CB2-OB2-PB2-OB3
56	P	501	NDP	O4B-C4B-C5B-O5B
48	B	203	PC1	O22-C21-C22-C23
46	b	901	3PE	O13-C11-C12-N
46	J	401	3PE	O32-C31-C32-C33
46	M	603	3PE	O22-C21-C22-C23
45	l	201	LMT	C5-C6-C7-C8
46	A	302	3PE	C12-C11-O13-P
46	H	601	3PE	C12-C11-O13-P
58	T	101	EHZ	C21-C1-C2-C3
45	L	702	LMT	C2-C3-C4-C5
46	J	401	3PE	C35-C36-C37-C38
45	L	705	LMT	C5-C6-C7-C8
53	q	201	CDL	C39-C40-C41-C42
46	I	201	3PE	C22-C23-C24-C25
46	J	401	3PE	O21-C21-C22-C23

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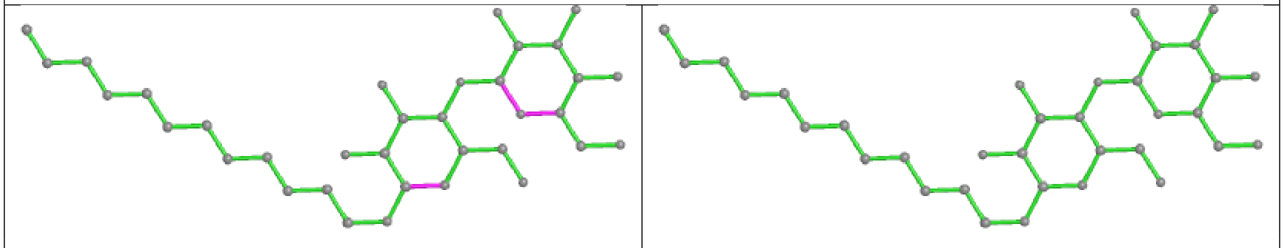
Mol	Chain	Res	Type	Atoms
50	F	501	FMN	N10-C1'-C2'-O2'
46	A	302	3PE	O32-C31-C32-C33
46	I	201	3PE	O32-C31-C32-C33
53	L	704	CDL	C52-C51-CB5-OB7
46	I	201	3PE	O31-C31-C32-C33
46	O	1201	3PE	O21-C21-C22-C23
53	q	201	CDL	C32-C31-CA7-OA8
46	O	1201	3PE	C34-C35-C36-C37
53	L	704	CDL	C64-C65-C66-C67
46	b	901	3PE	O22-C21-C22-C23
53	q	201	CDL	C32-C31-CA7-OA9
46	L	703	3PE	C33-C34-C35-C36
45	M	606	LMT	C2-C1-O1'-C1'
46	M	603	3PE	C3B-C3C-C3D-C3E
46	J	401	3PE	O22-C21-C22-C23
46	M	603	3PE	C23-C24-C25-C26

There are no ring outliers.

No monomer is involved in short contacts.

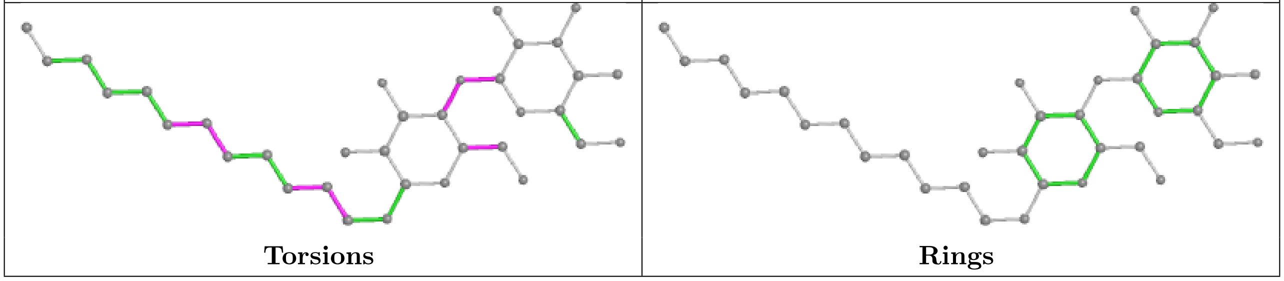
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand LMT l 201



Bond lengths

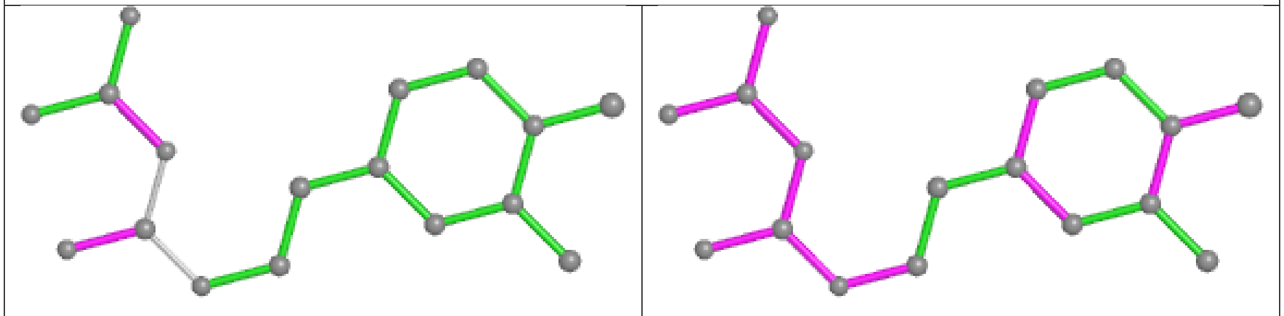
Bond angles



Torsions

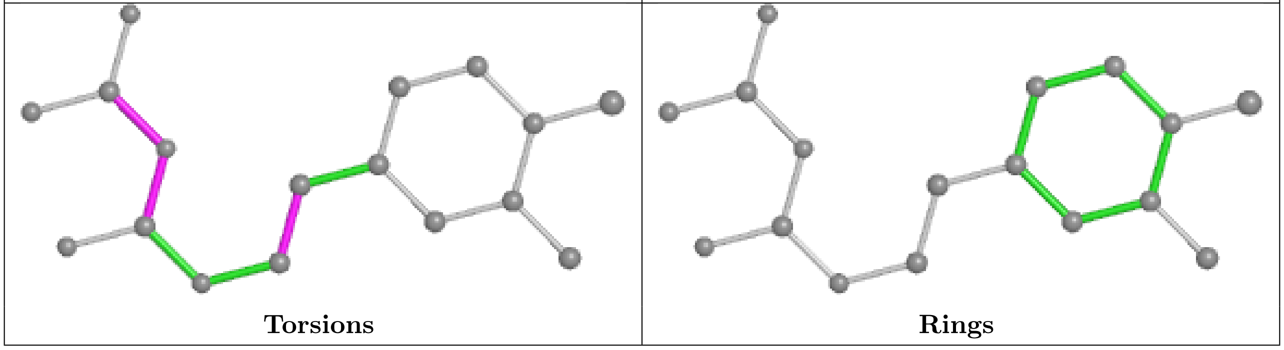
Rings

Ligand I49 H 602



Bond lengths

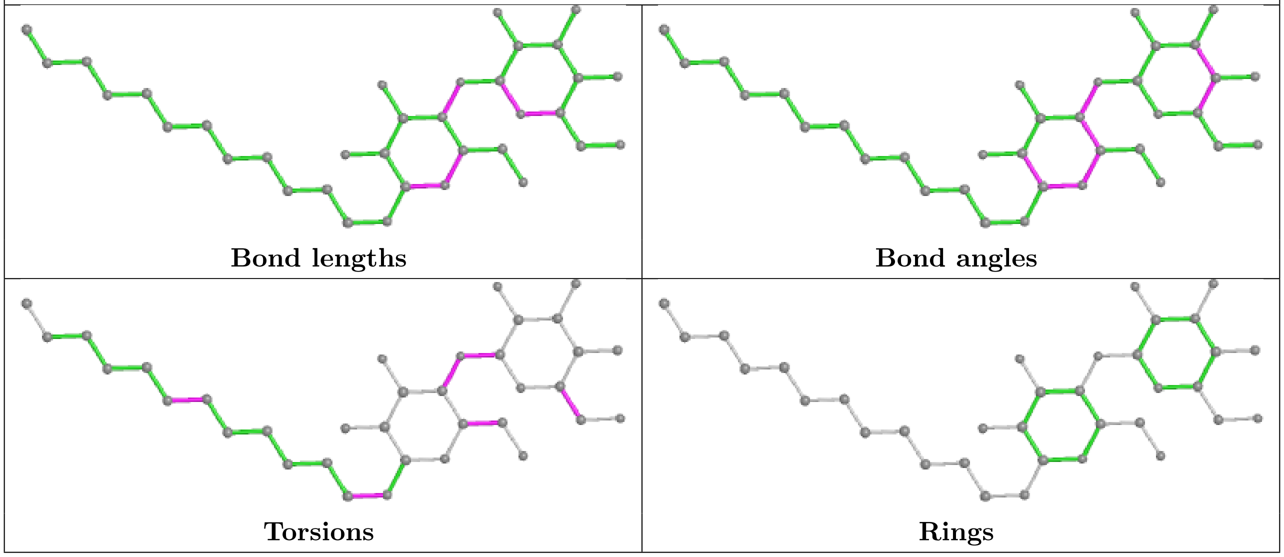
Bond angles



Torsions

Rings

Ligand LMT M 606



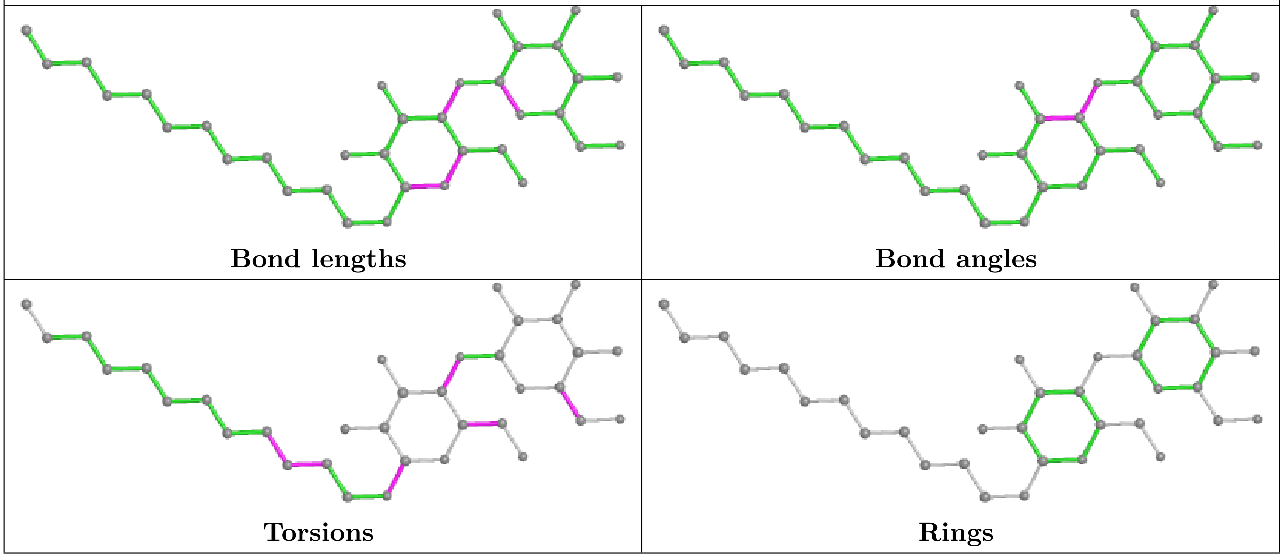
Bond lengths

Bond angles

Torsions

Rings

Ligand LMT A 301



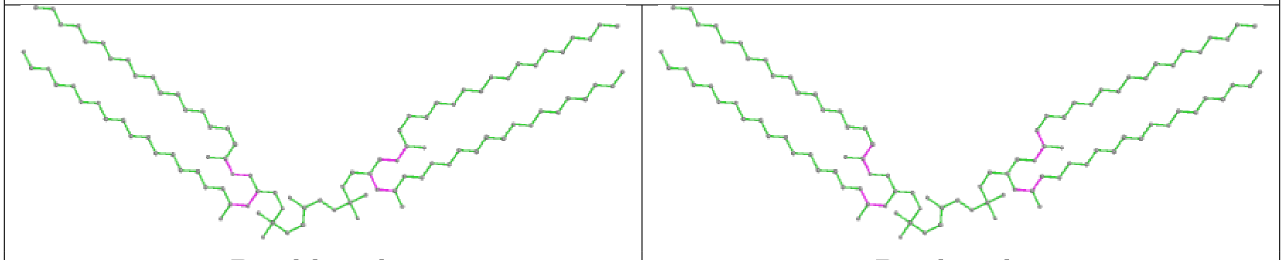
Bond lengths

Bond angles

Torsions

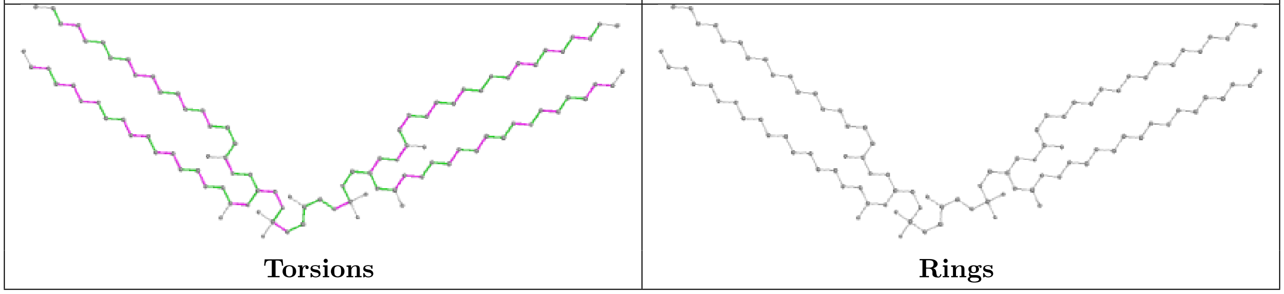
Rings

Ligand CDL L 704



Bond lengths

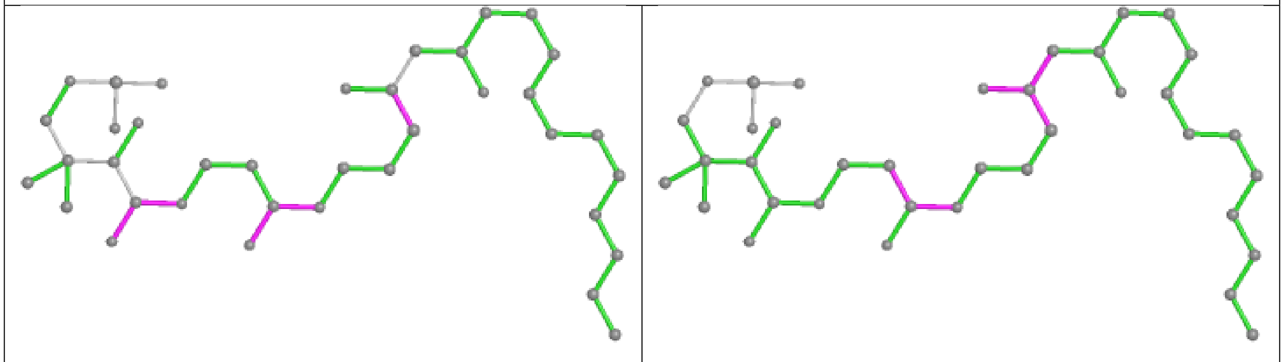
Bond angles



Torsions

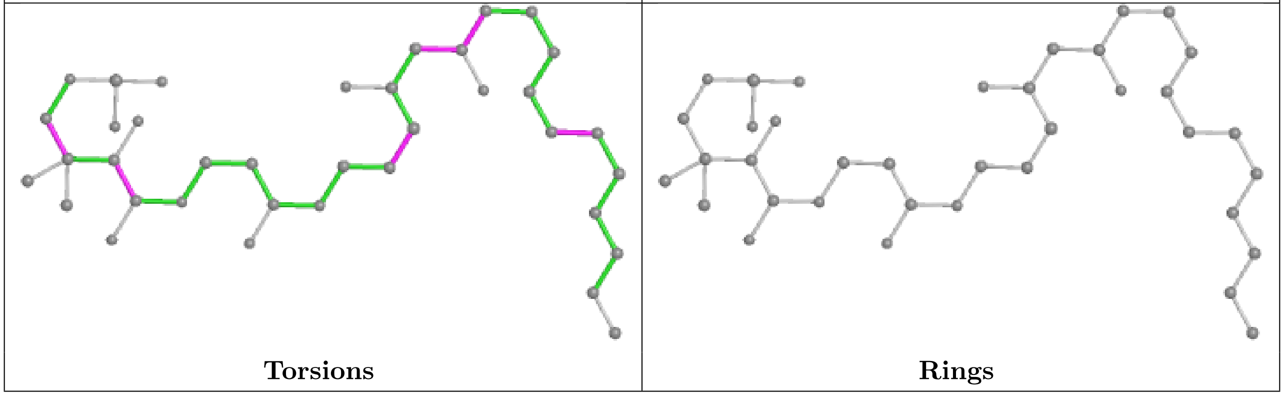
Rings

Ligand EHZ T 101



Bond lengths

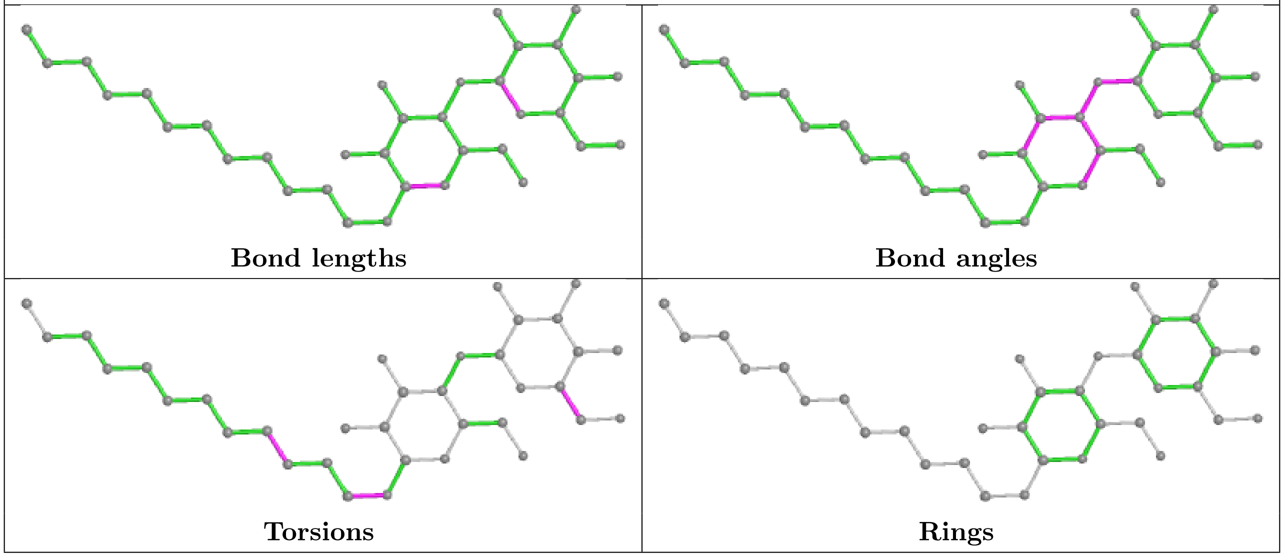
Bond angles



Torsions

Rings

Ligand LMT h 1002



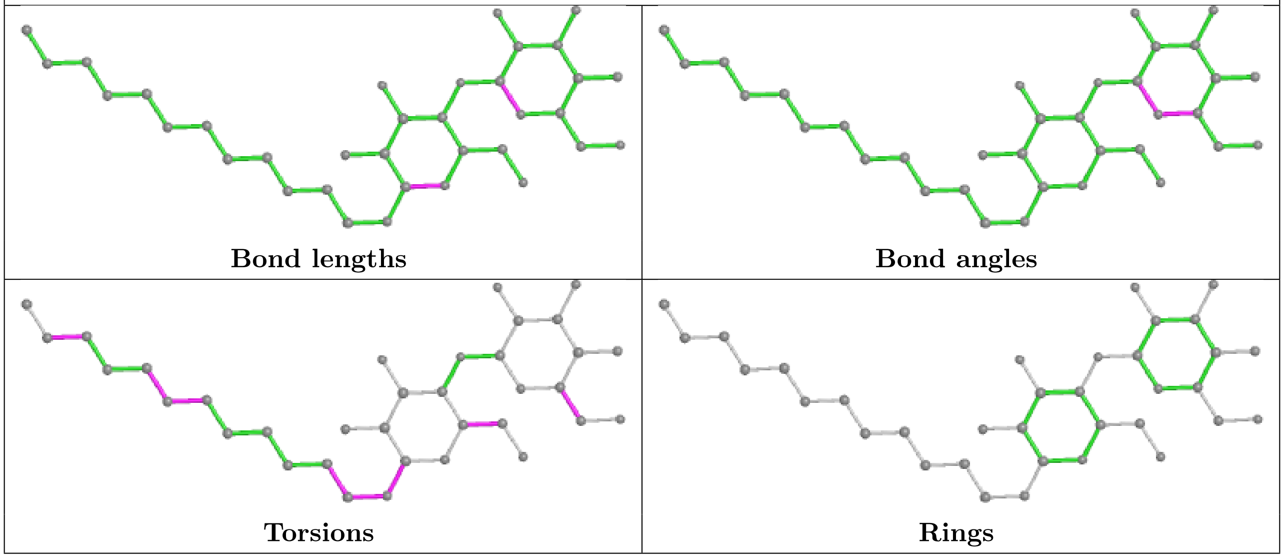
Bond lengths

Bond angles

Torsions

Rings

Ligand LMT L 706



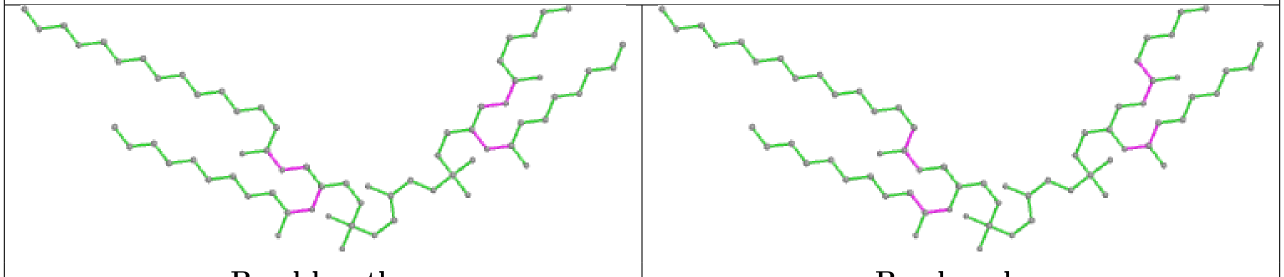
Bond lengths

Bond angles

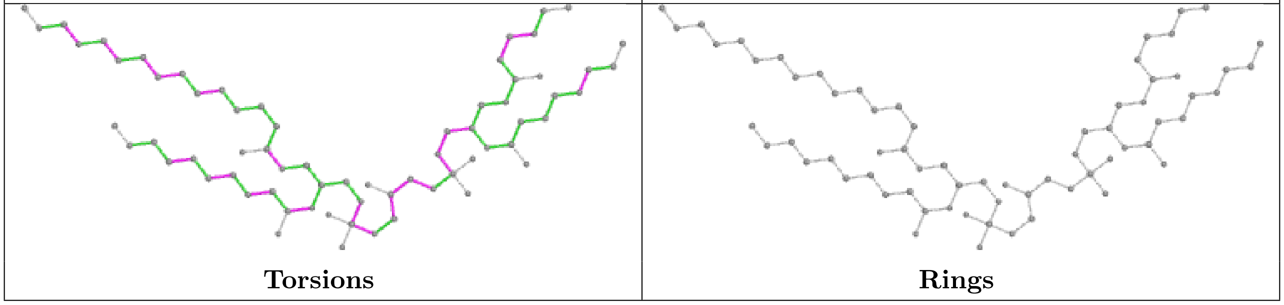
Torsions

Rings

Ligand CDL K 401

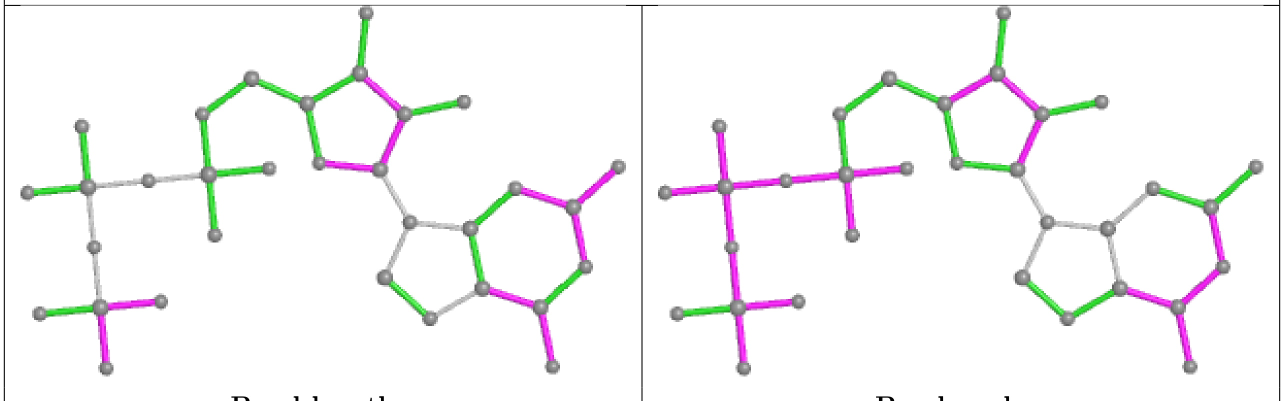


Bond lengths **Bond angles**

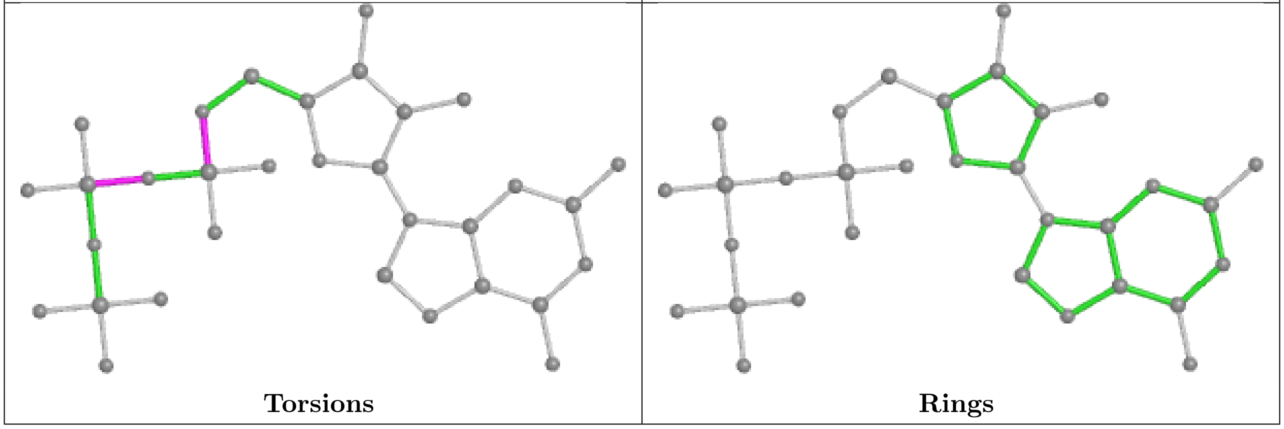


Torsions **Rings**

Ligand GTP O 1202

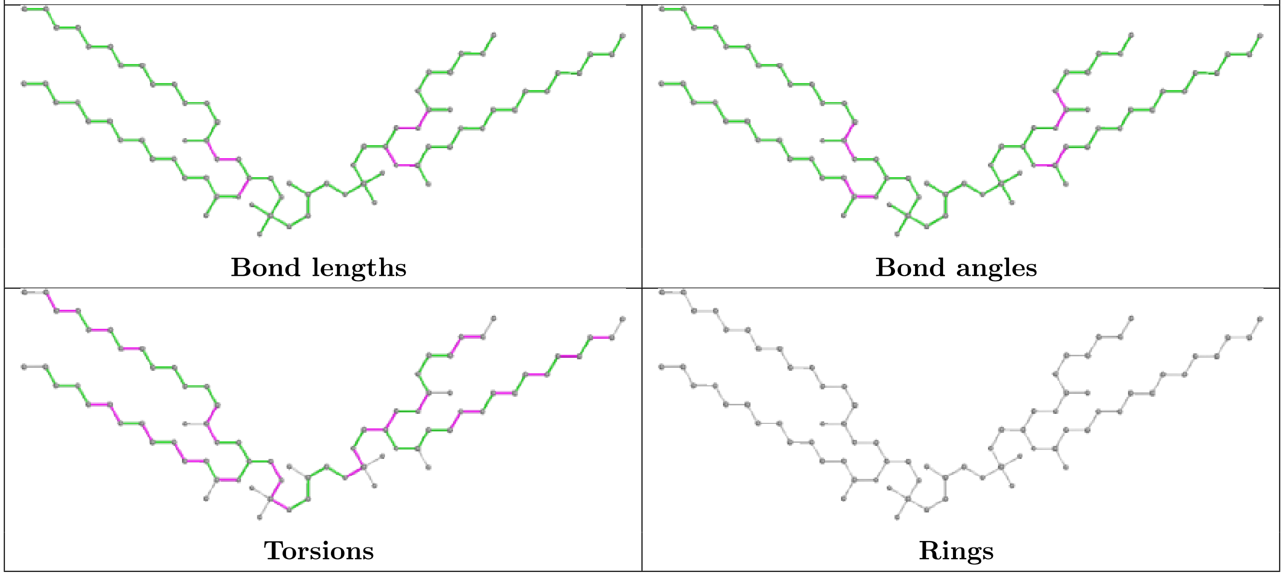


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CDL q 201



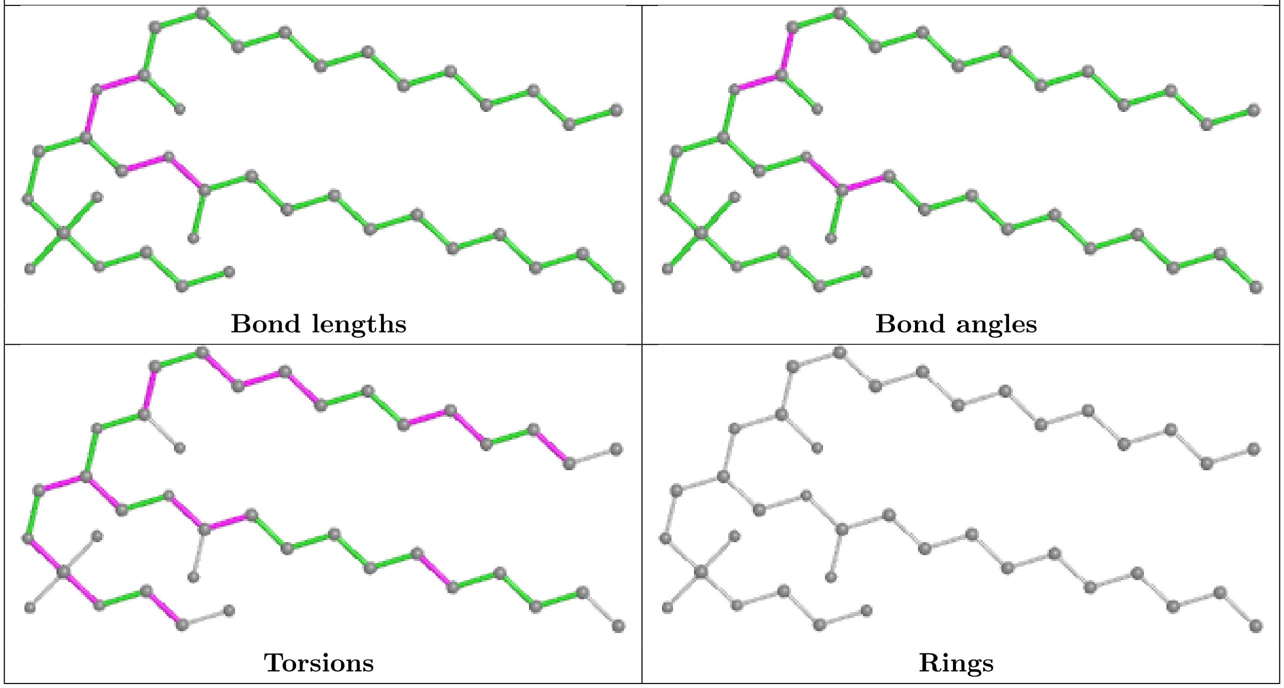
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE b 901



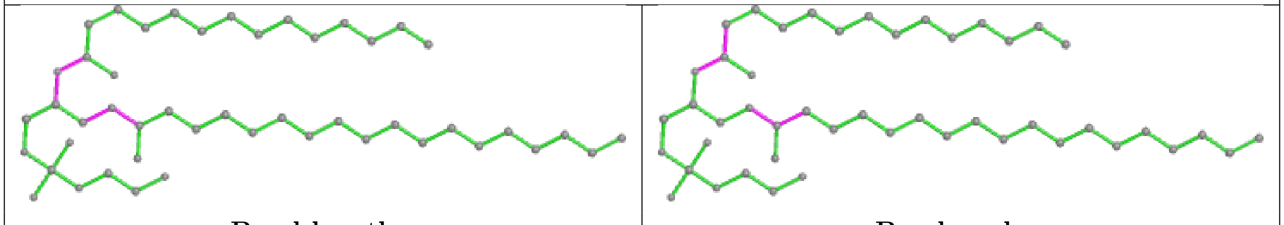
Bond lengths

Bond angles

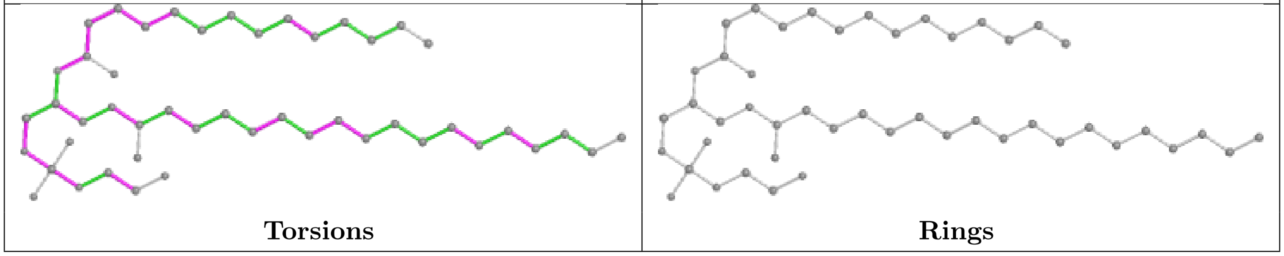
Torsions

Rings

Ligand 3PE O 1201

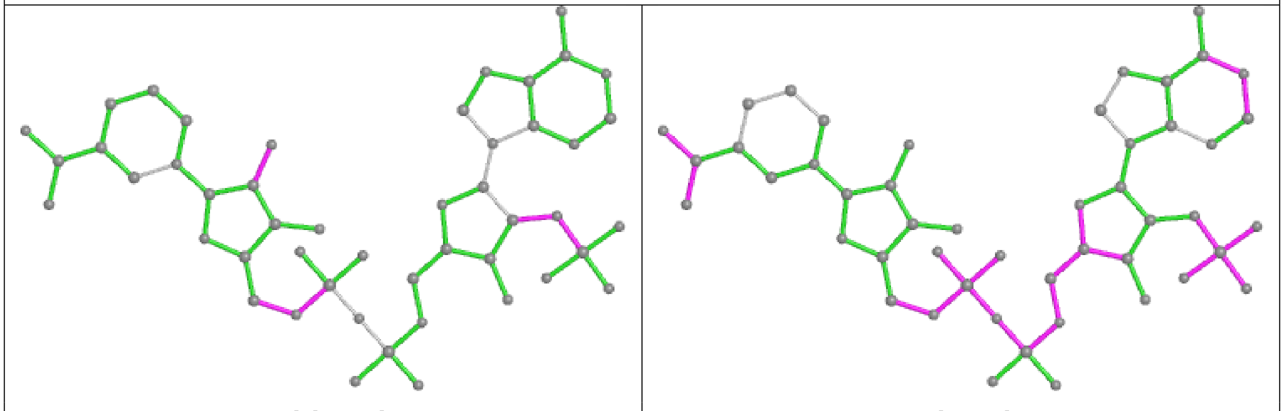


Bond lengths **Bond angles**

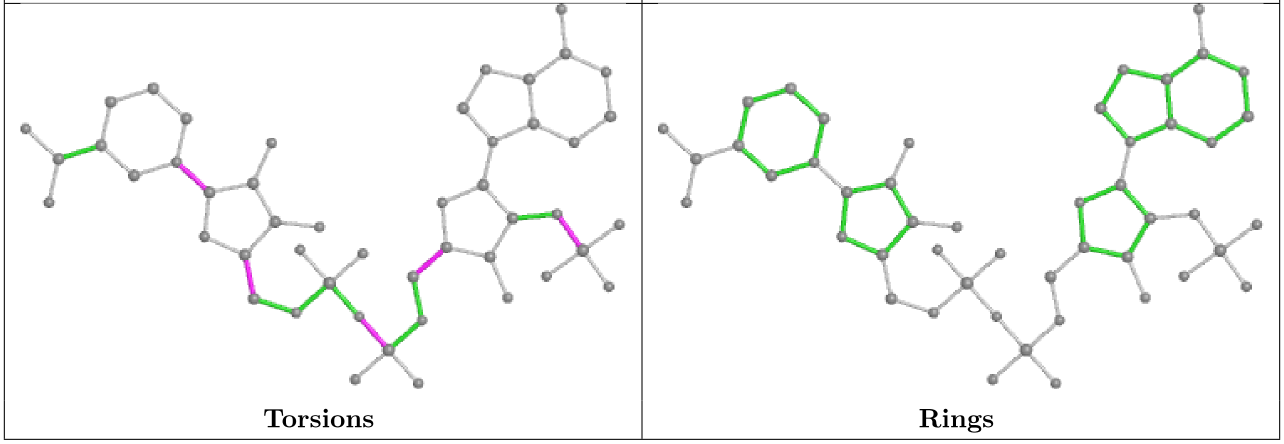


Torsions **Rings**

Ligand NDP P 501

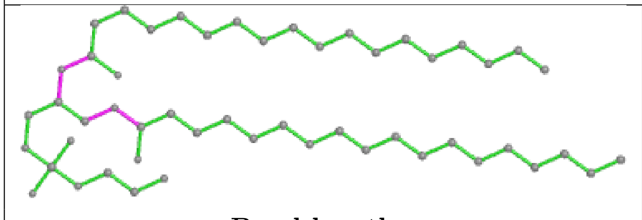


Bond lengths **Bond angles**

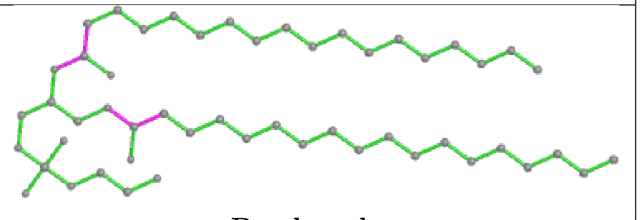


Torsions **Rings**

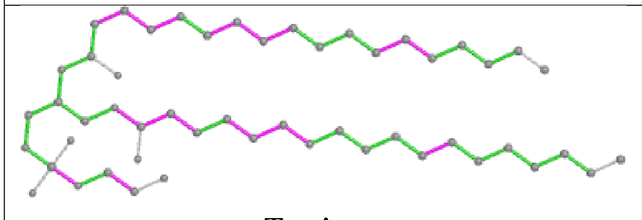
Ligand 3PE I 201



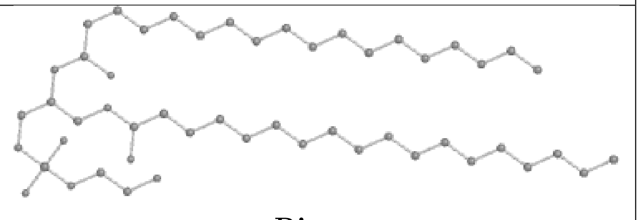
Bond lengths



Bond angles

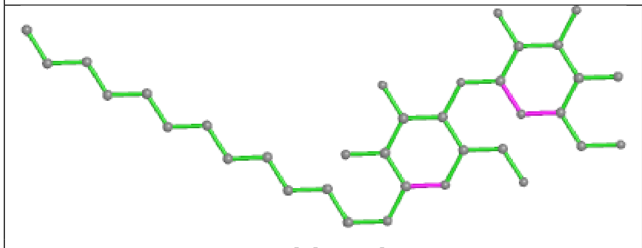


Torsions

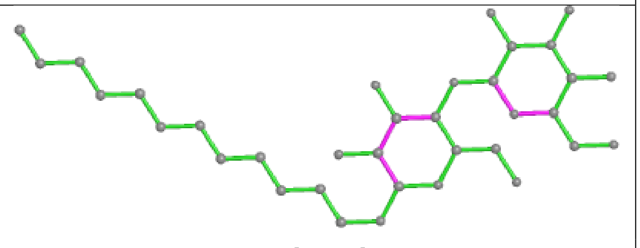


Rings

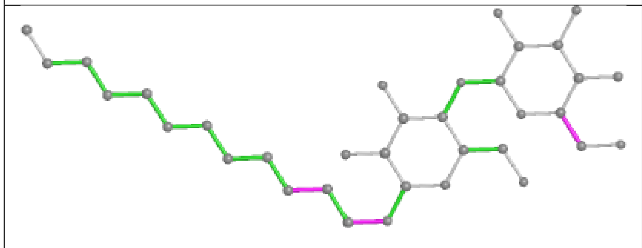
Ligand LMT M 602



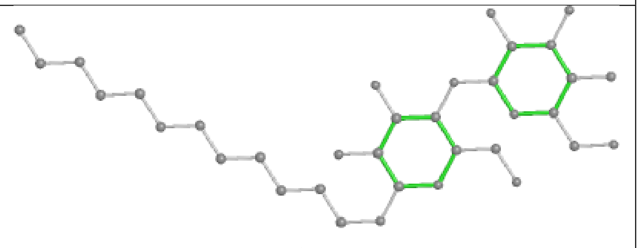
Bond lengths



Bond angles

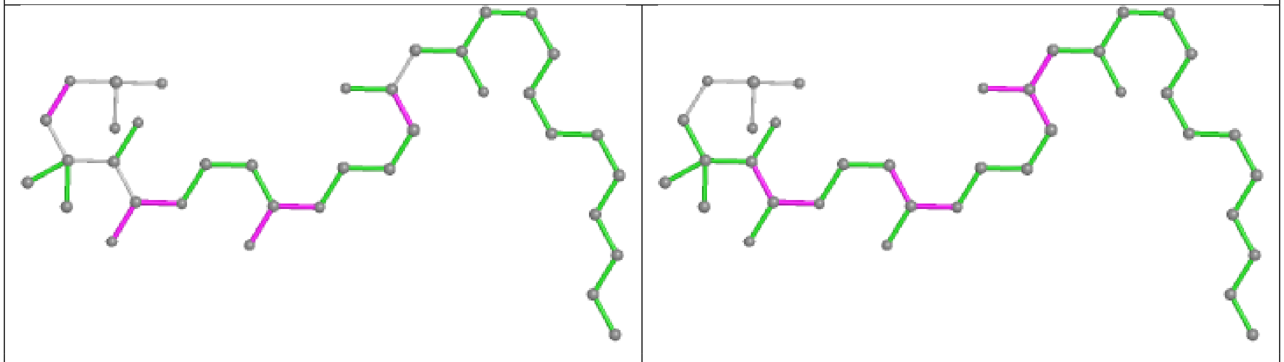


Torsions



Rings

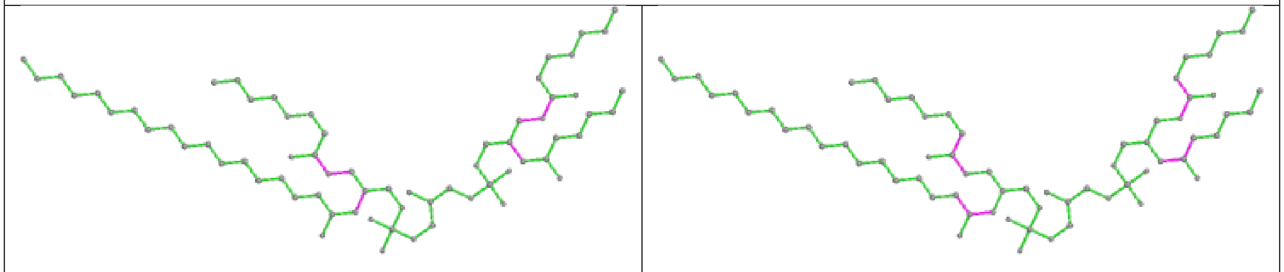
Ligand EHZ U 101



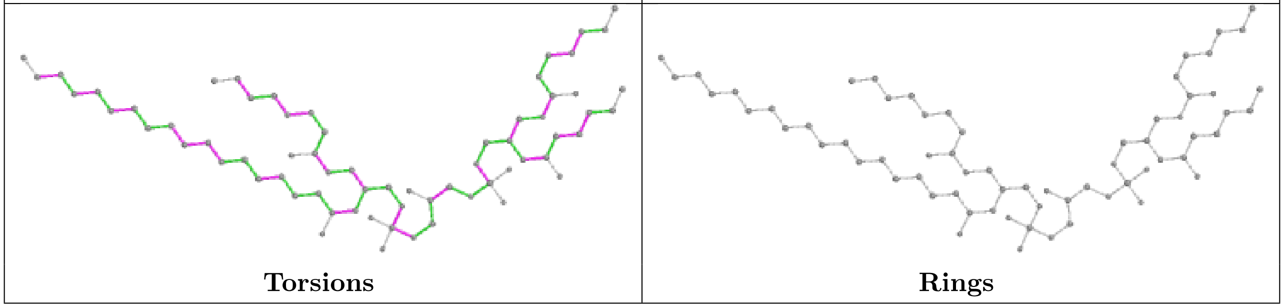
Bond lengths **Bond angles**

Torsions **Rings**

Ligand CDL h 1001

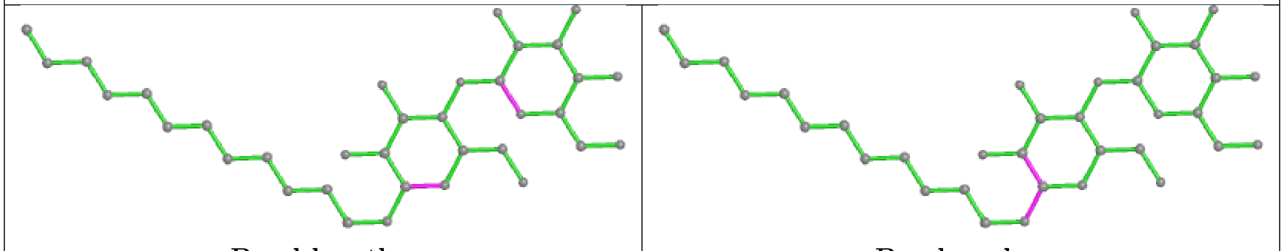


Bond lengths **Bond angles**



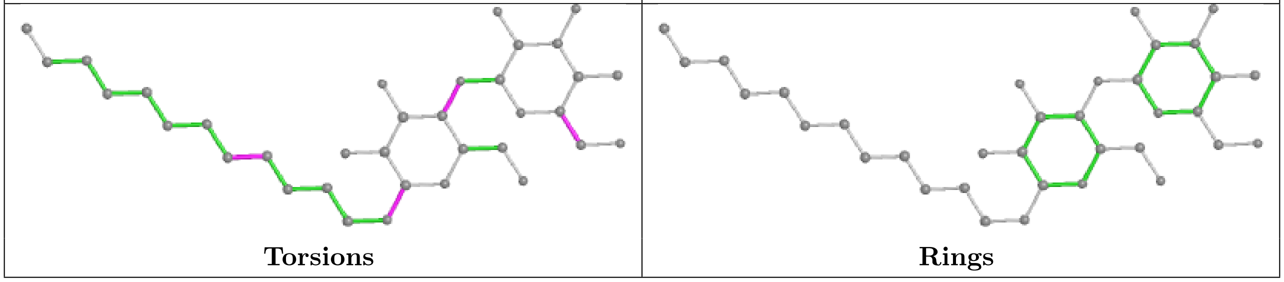
Torsions **Rings**

Ligand LMT B 202



Bond lengths

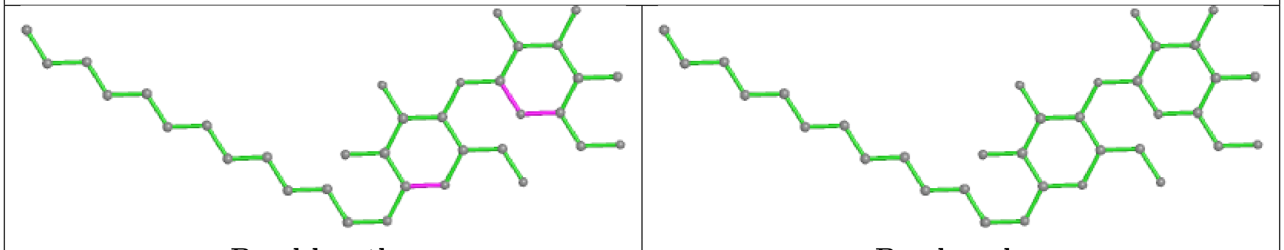
Bond angles



Torsions

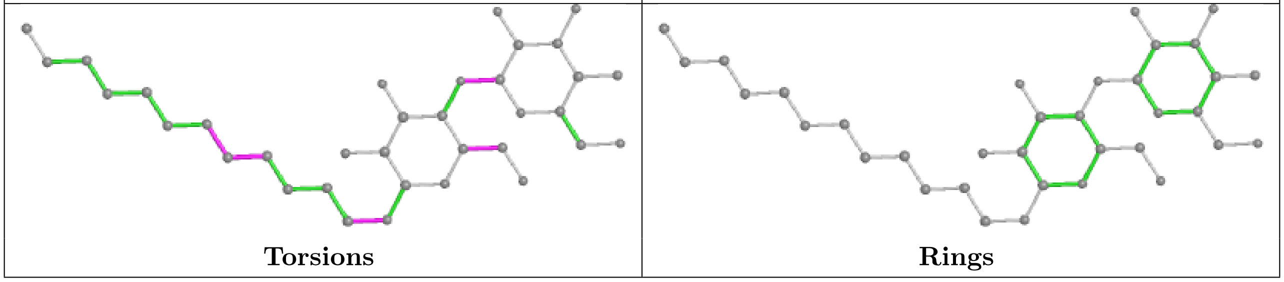
Rings

Ligand LMT J 402



Bond lengths

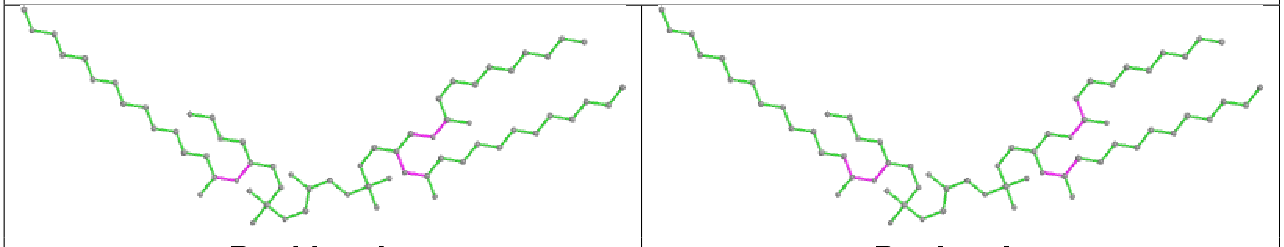
Bond angles



Torsions

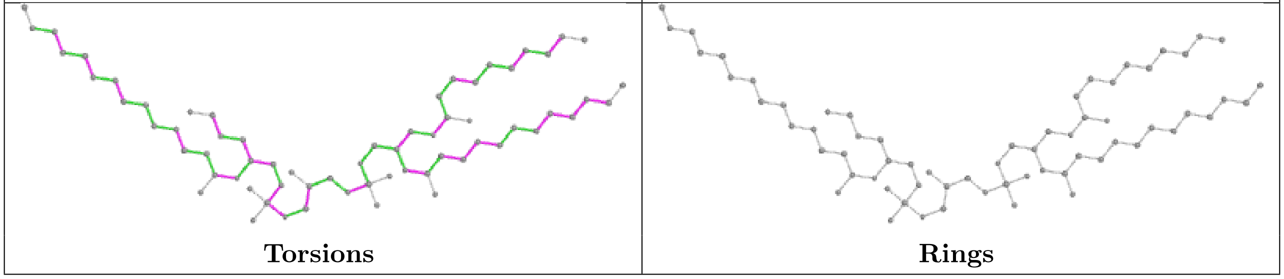
Rings

Ligand CDL X 1701



Bond lengths

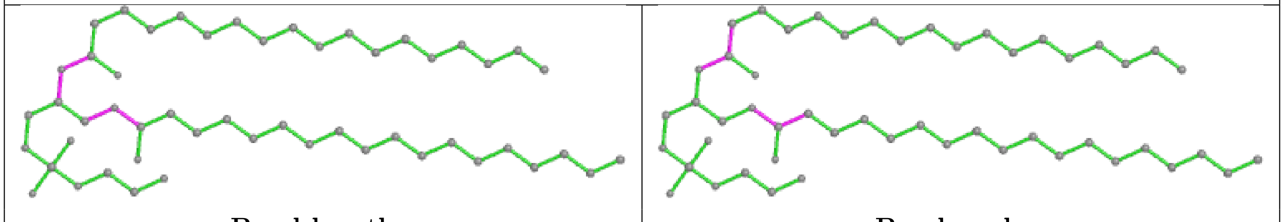
Bond angles



Torsions

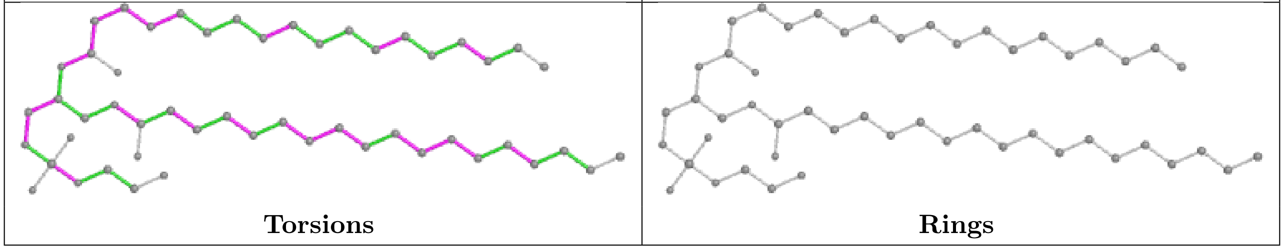
Rings

Ligand 3PE M 603



Bond lengths

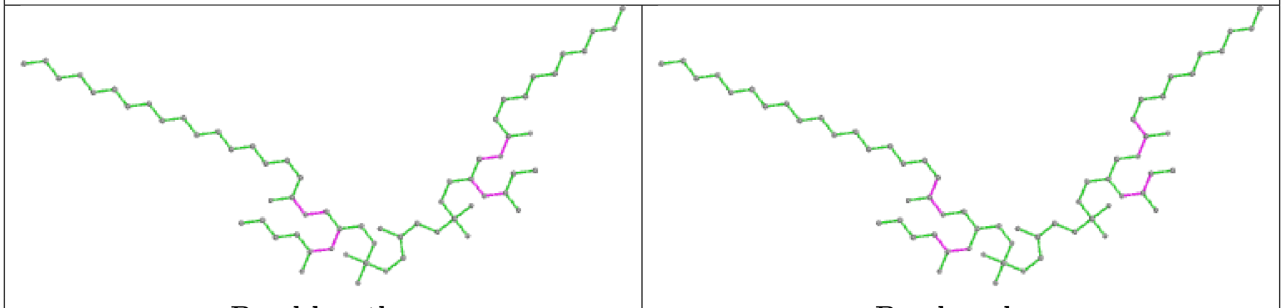
Bond angles



Torsions

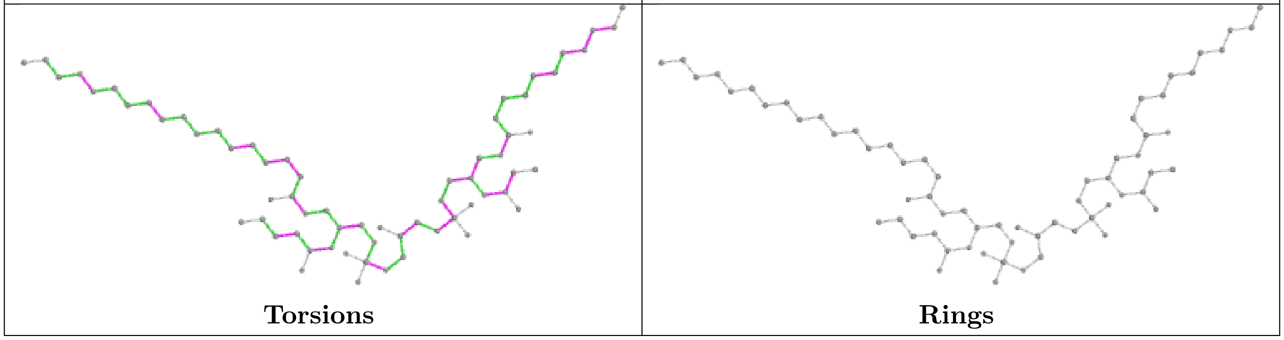
Rings

Ligand CDL d 201



Bond lengths

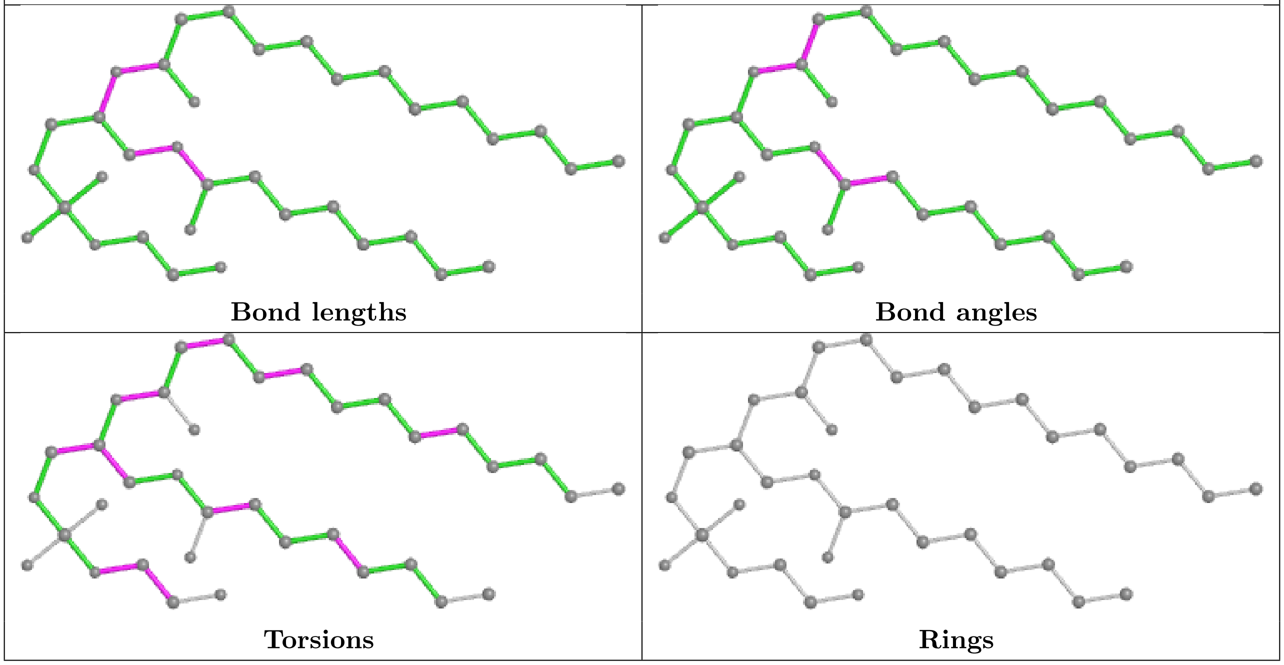
Bond angles



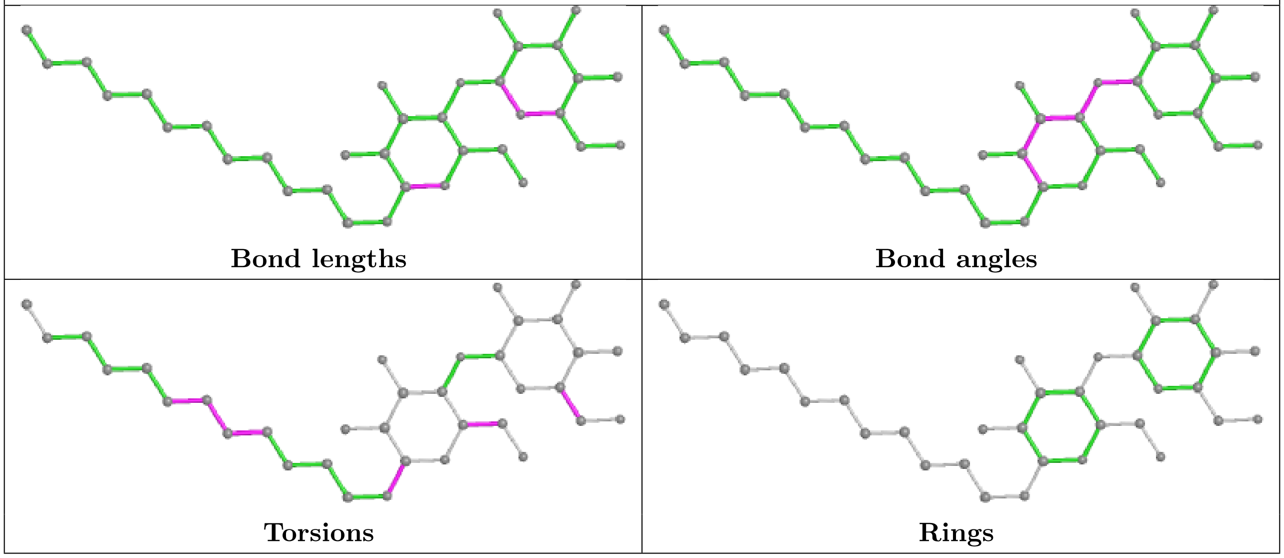
Torsions

Rings

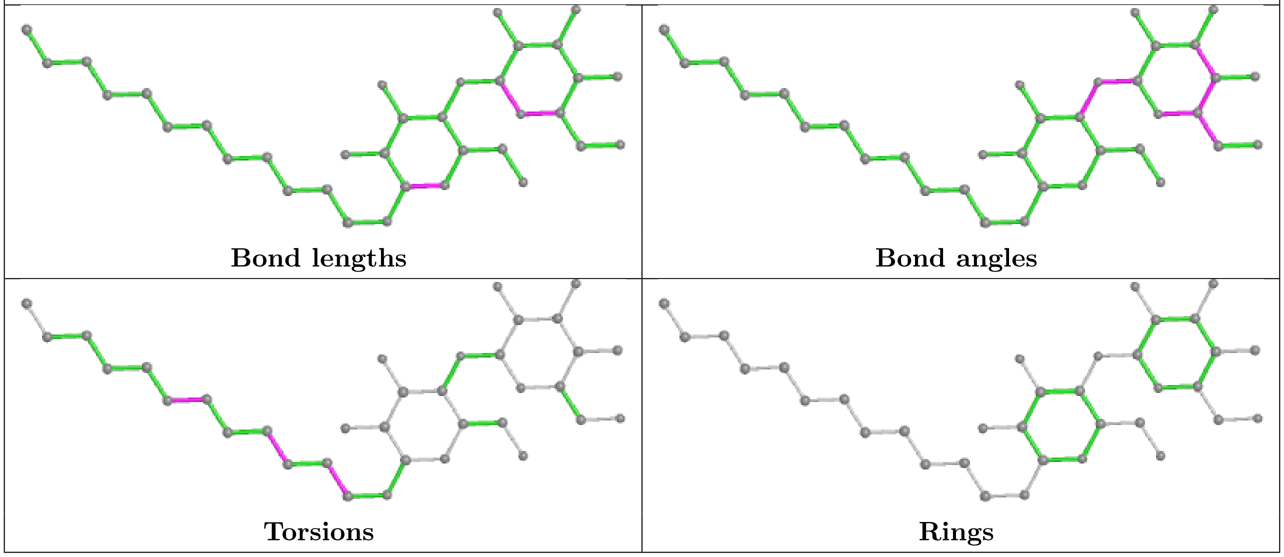
Ligand 3PE A 302



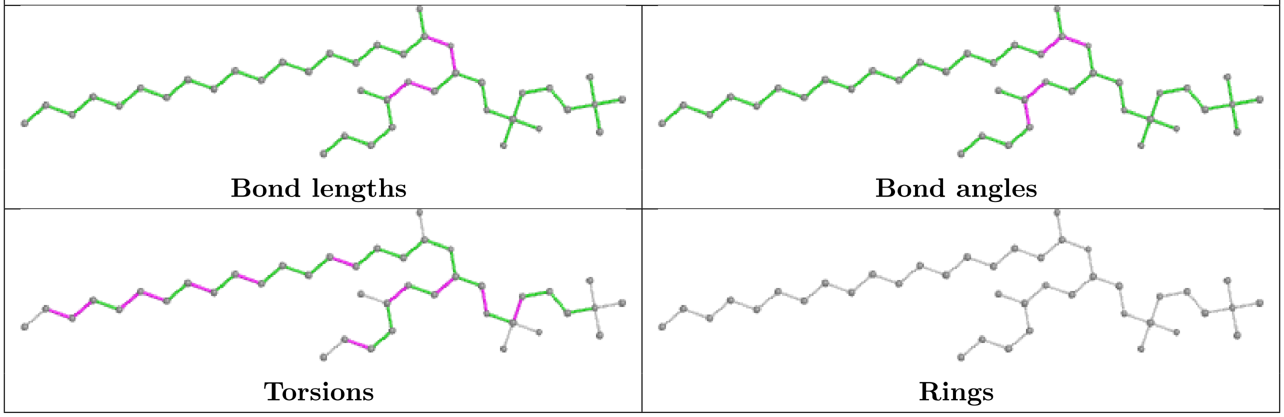
Ligand LMT L 705



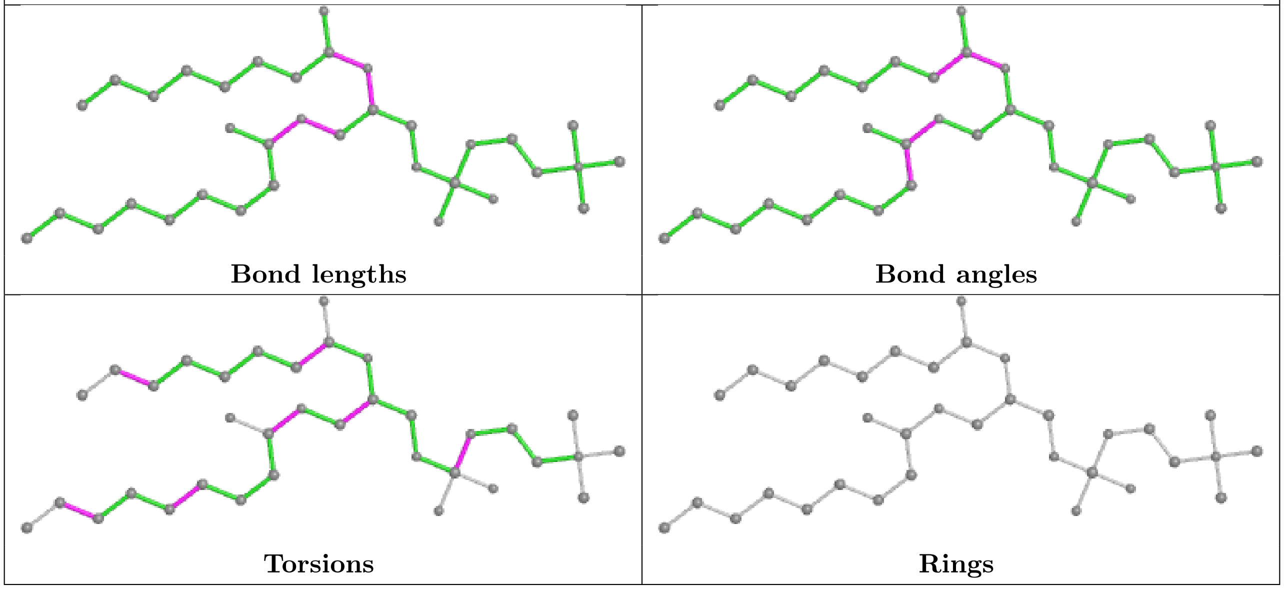
Ligand LMT L 702



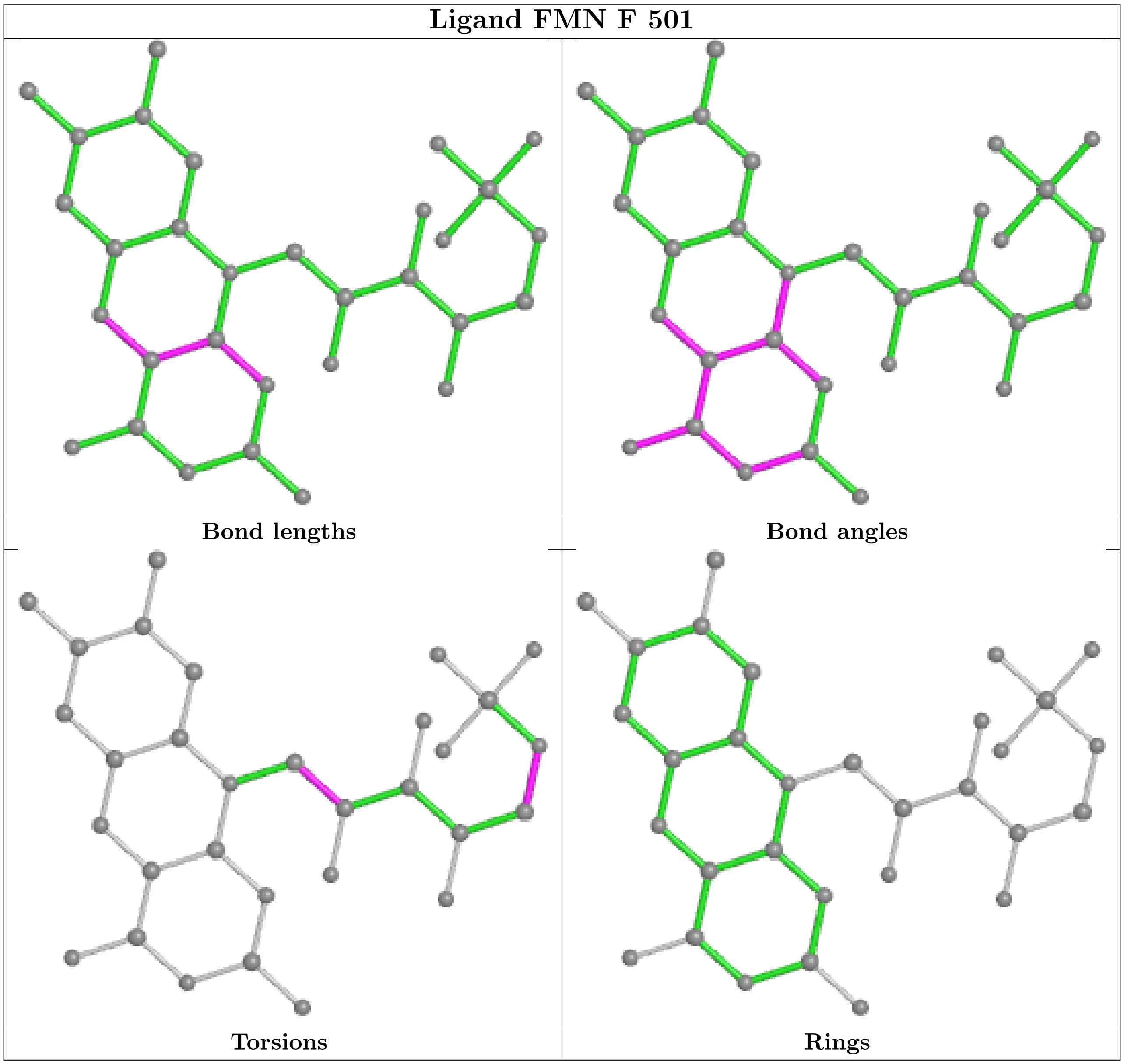
Ligand PC1 M 604



Ligand PC1 B 203



Ligand FMN F 501



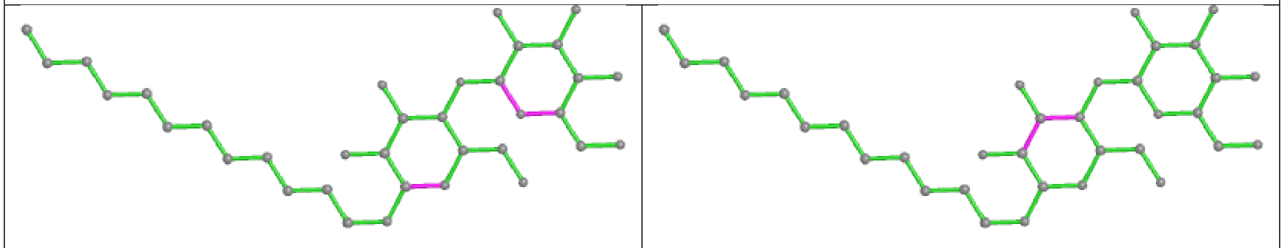
Bond lengths

Bond angles

Torsions

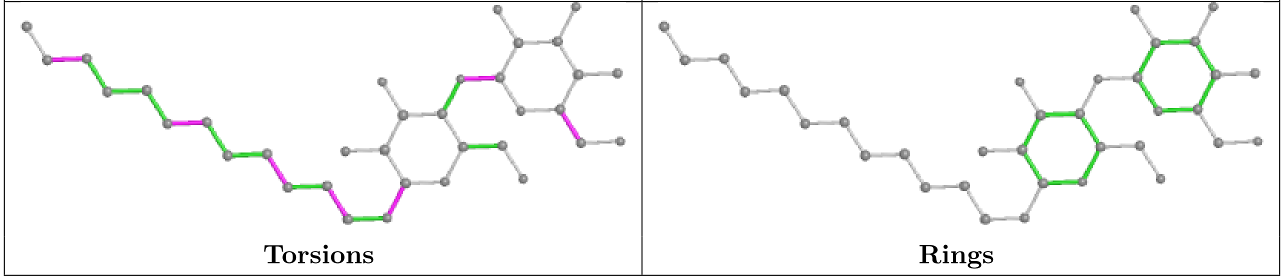
Rings

Ligand LMT M 605



Bond lengths

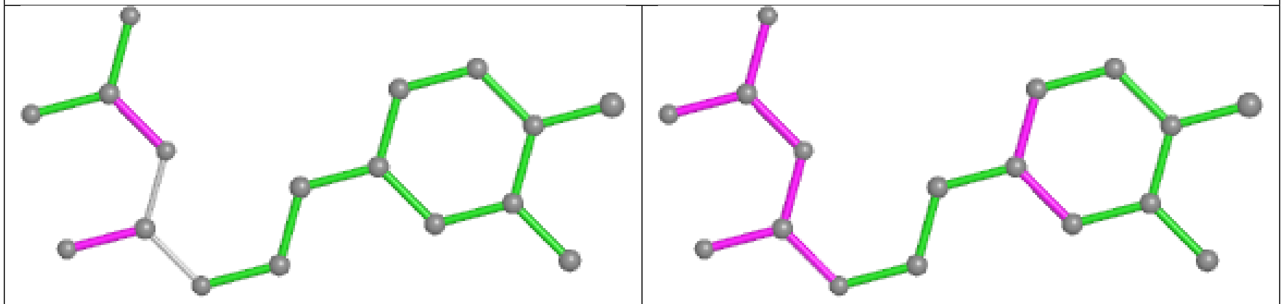
Bond angles



Torsions

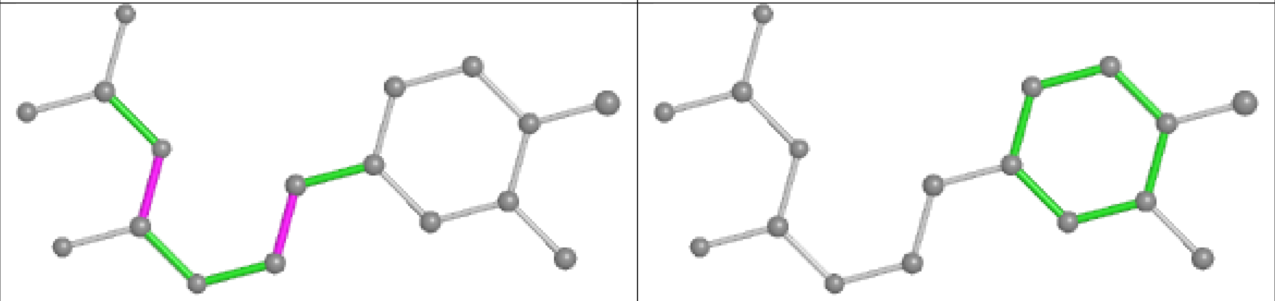
Rings

Ligand I49 N 503



Bond lengths

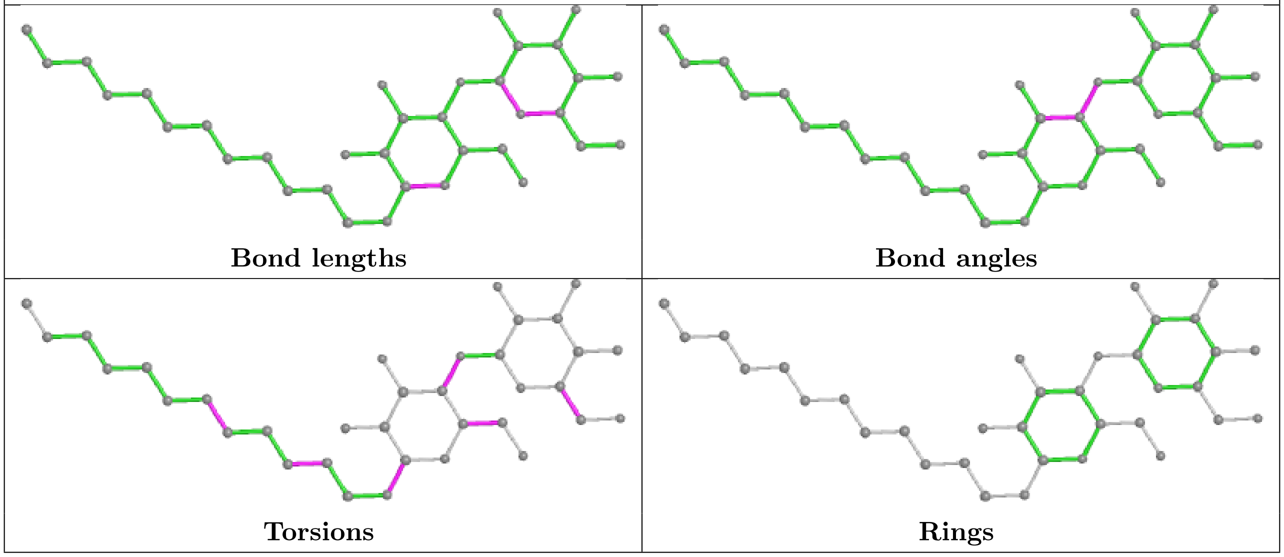
Bond angles



Torsions

Rings

Ligand LMT N 501



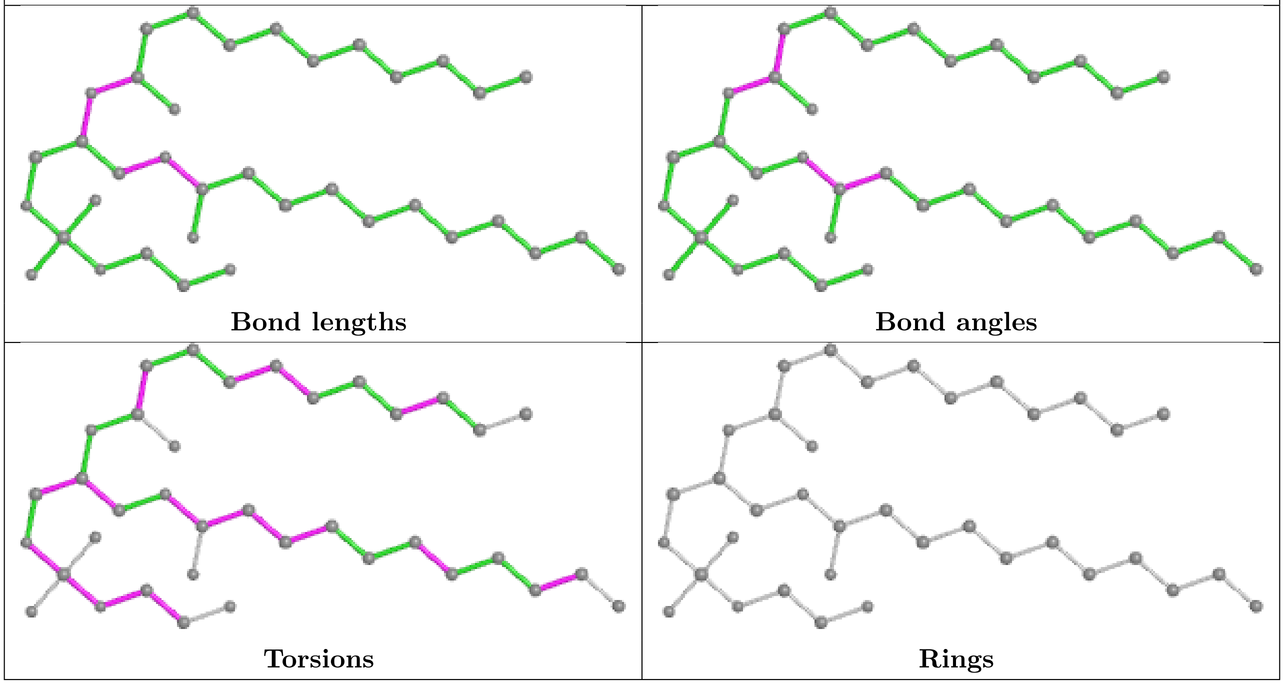
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE J 401



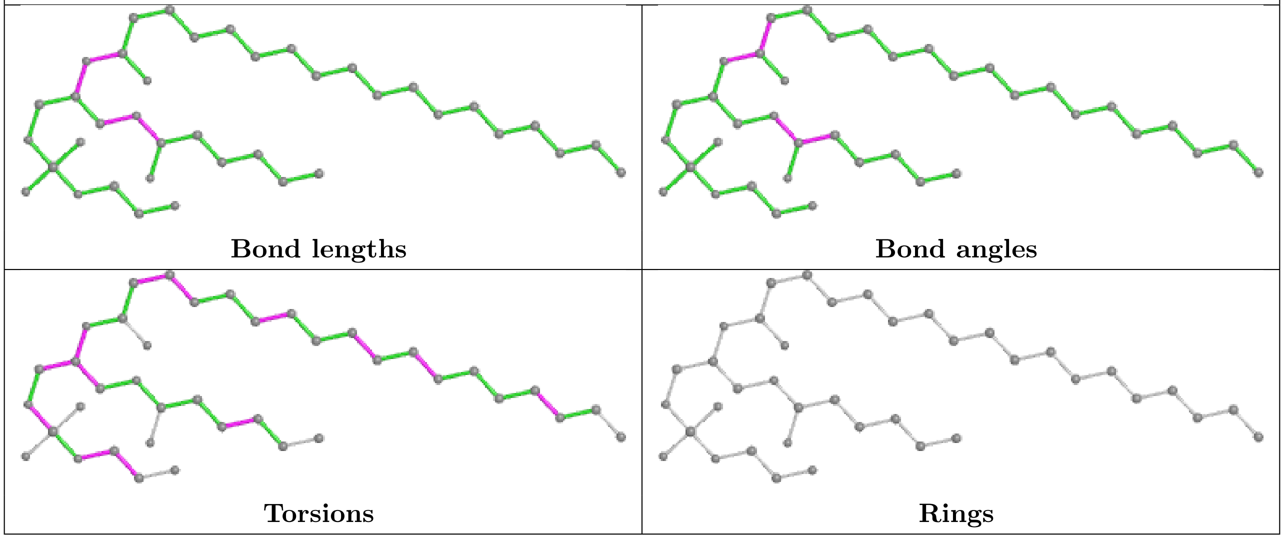
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE M 601



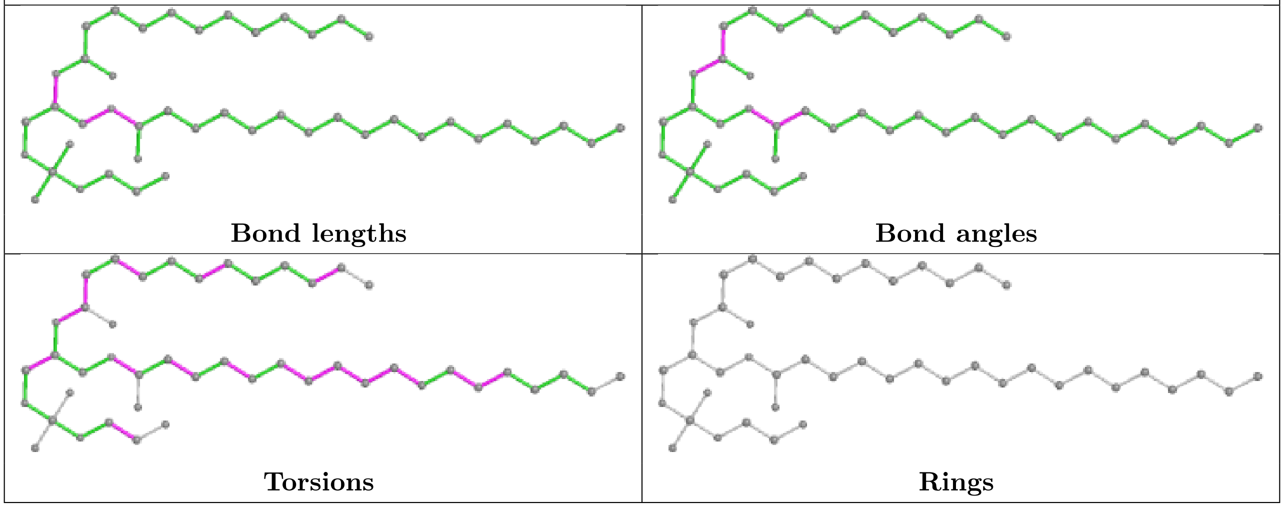
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE L 703



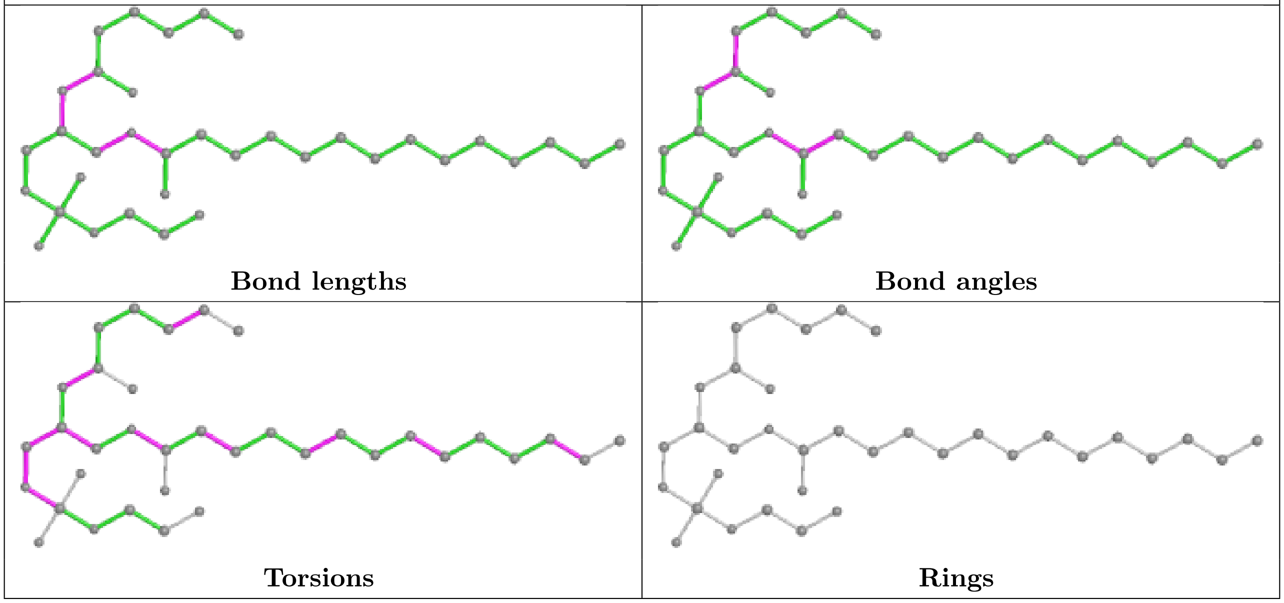
Bond lengths

Bond angles

Torsions

Rings

Ligand 3PE Y 401



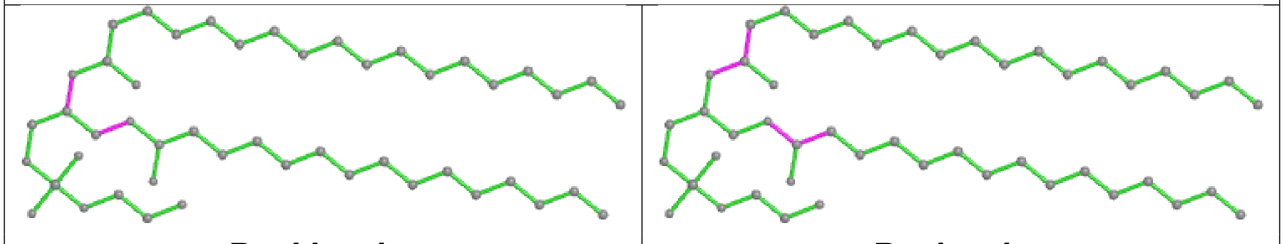
Bond lengths

Bond angles

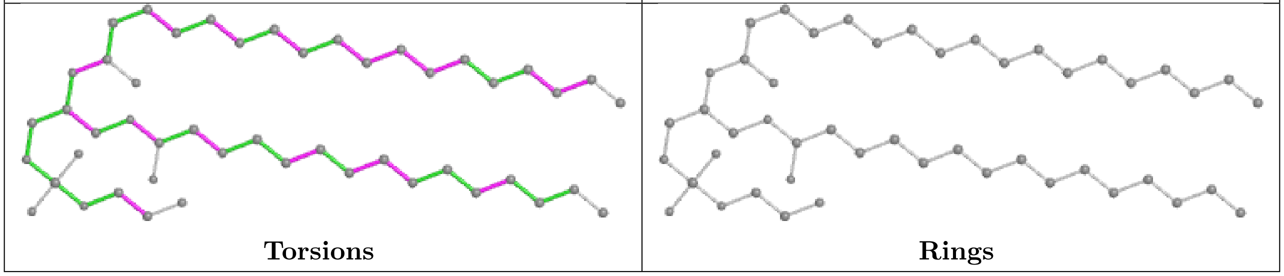
Torsions

Rings

Ligand 3PE L 701

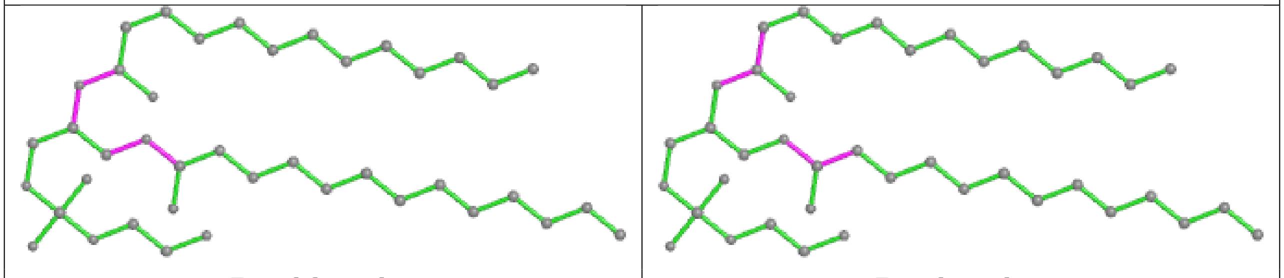


Bond lengths Bond angles

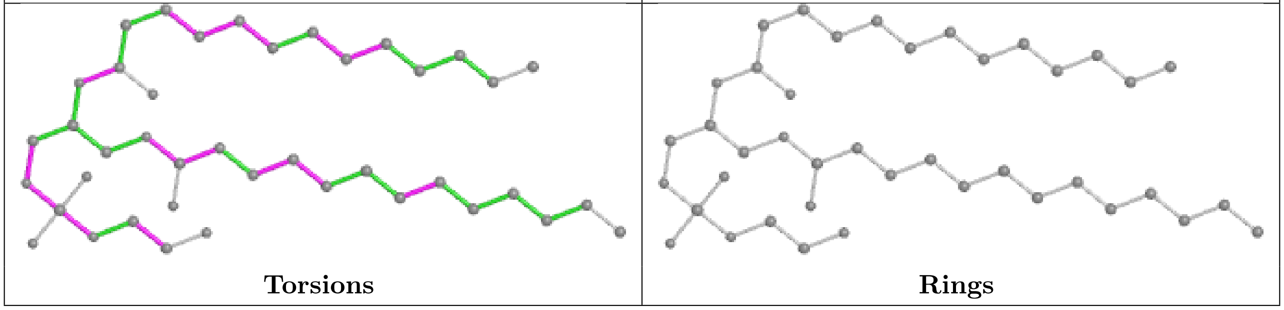


Torsions Rings

Ligand 3PE N 502

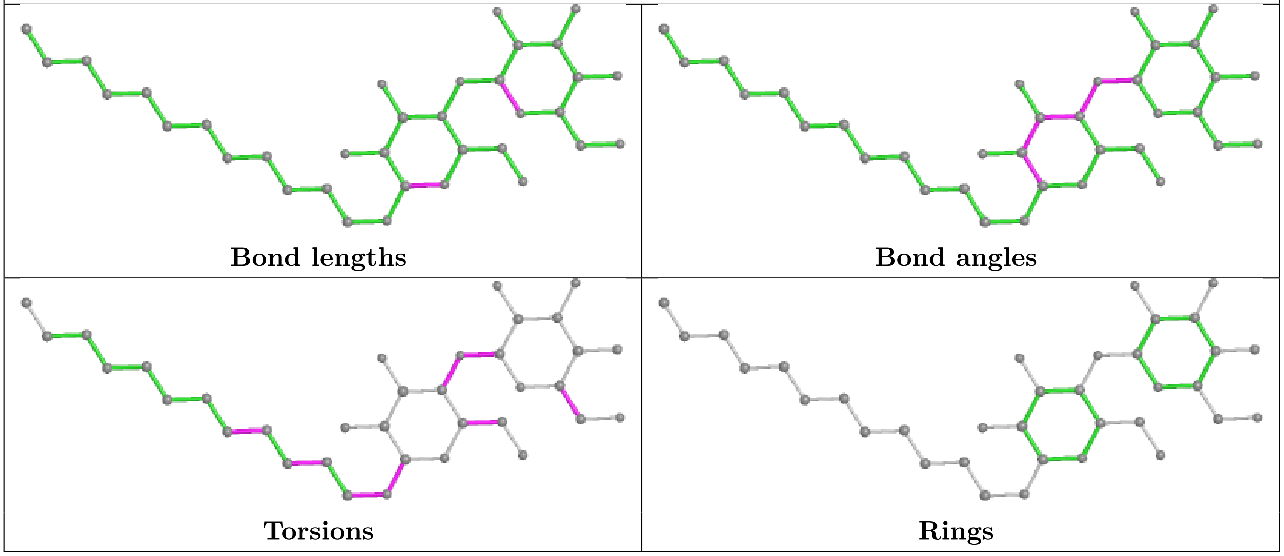


Bond lengths Bond angles

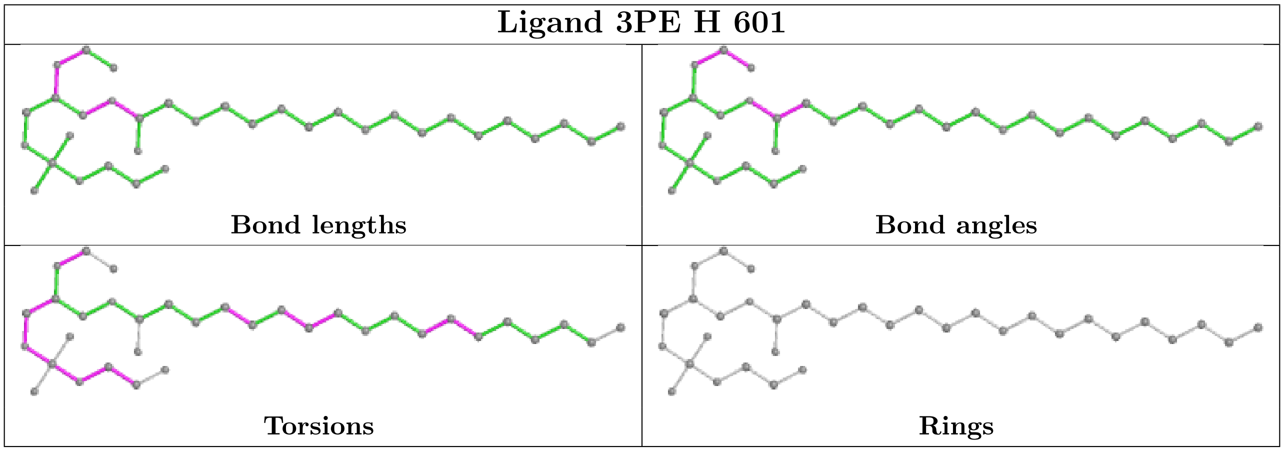


Torsions Rings

Ligand LMT f 1901



Ligand 3PE H 601



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

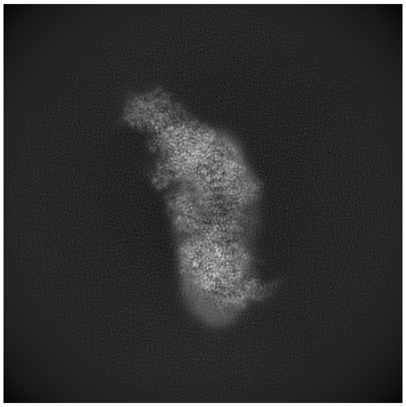
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14272. These allow visual inspection of the internal detail of the map and identification of artifacts.

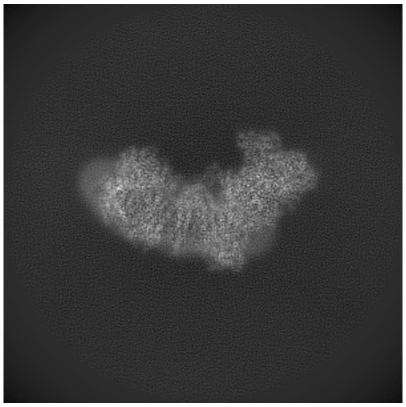
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

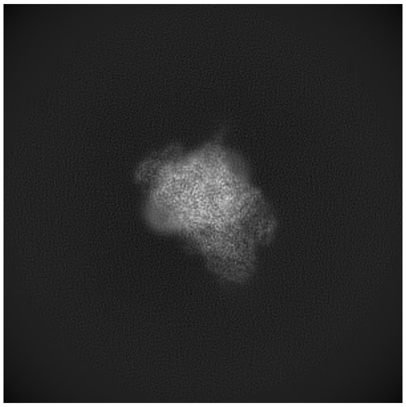
6.1.1 Primary map



X



Y

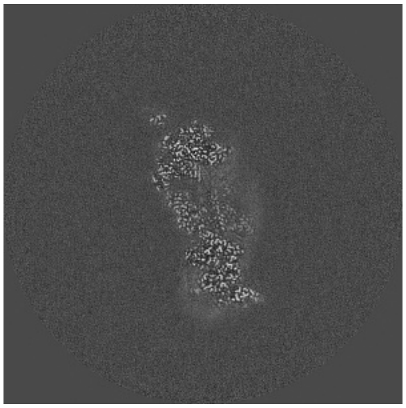


Z

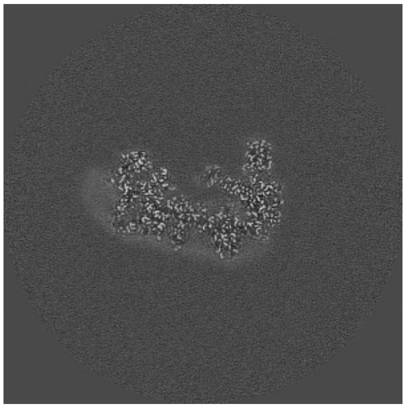
The images above show the map projected in three orthogonal directions.

6.2 Central slices

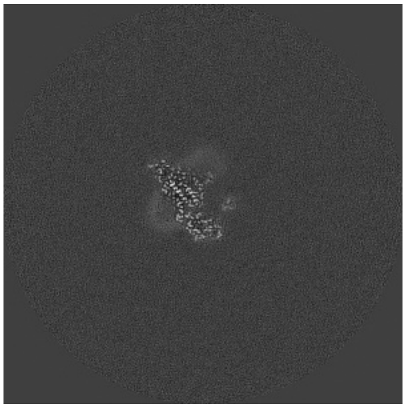
6.2.1 Primary map



X Index: 330



Y Index: 330

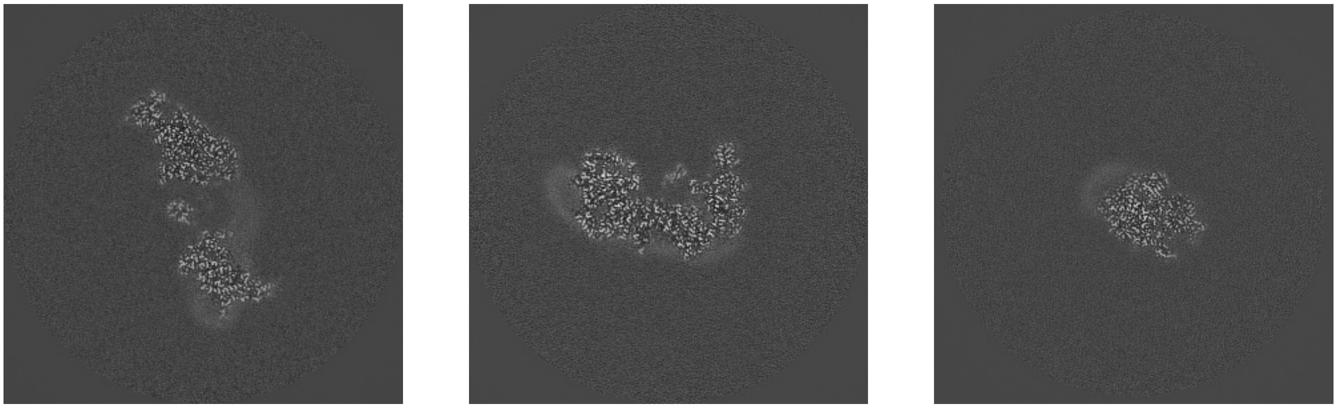


Z Index: 330

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map

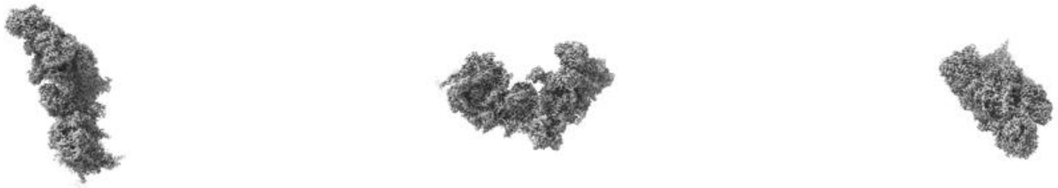


X Index: 356 Y Index: 338 Z Index: 422

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

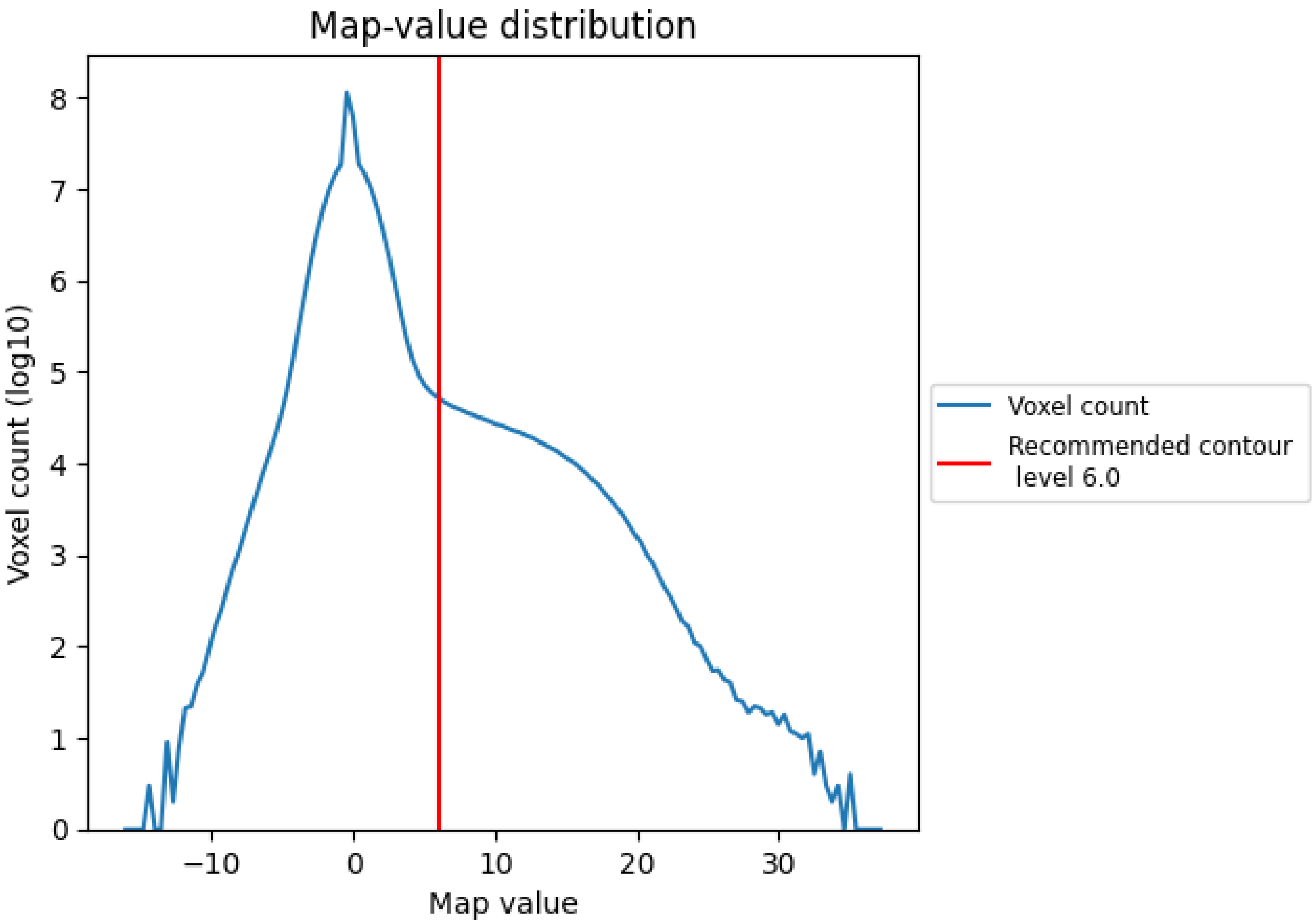
6.5 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

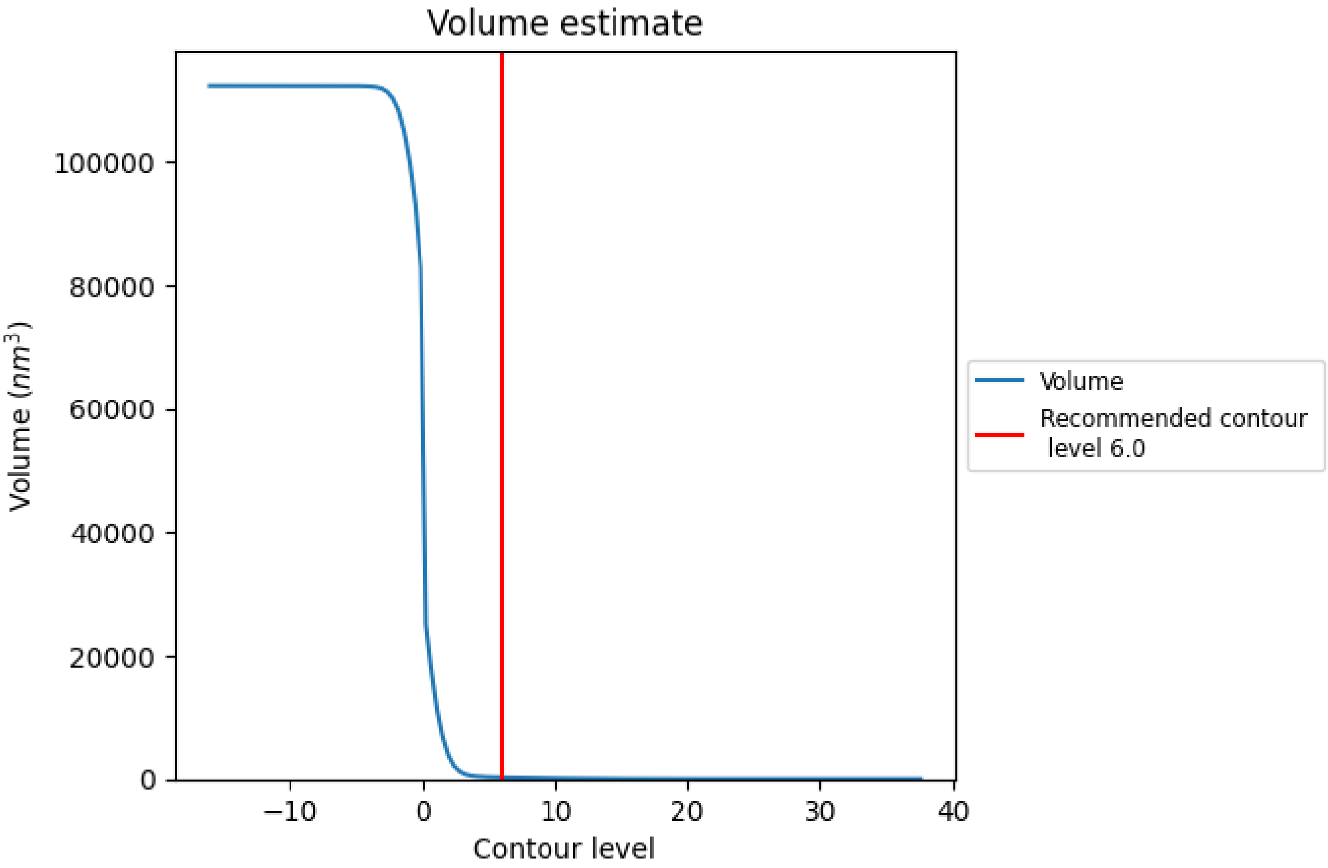
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

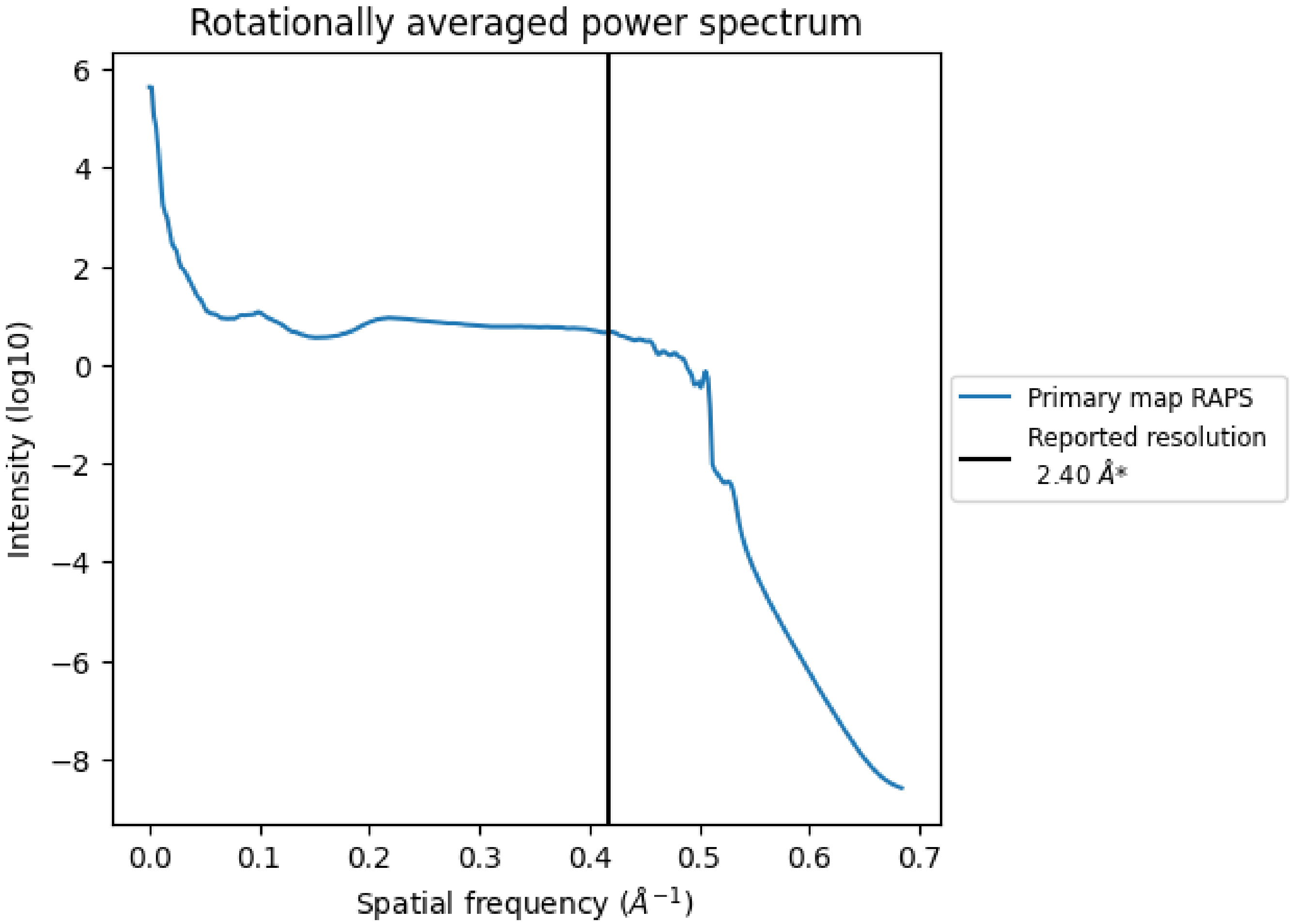
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 265 nm^3; this corresponds to an approximate mass of 240 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.417 $Å^{-1}$

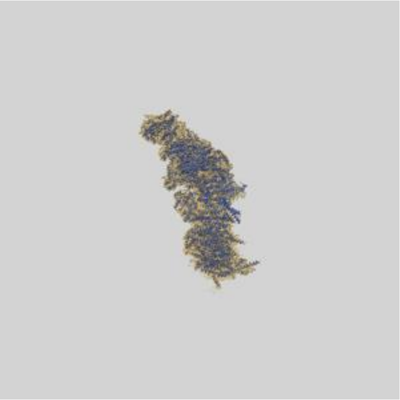
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

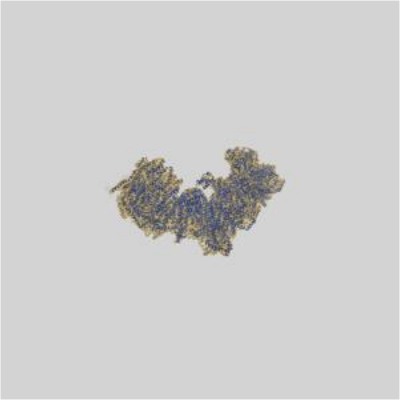
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-14272 and PDB model 7R45. Per-residue inclusion information can be found in section 3 on page 24.

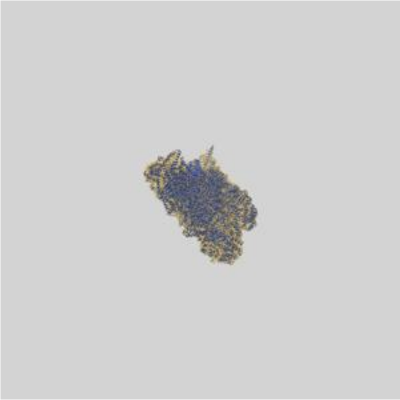
9.1 Map-model overlay ⓘ



X



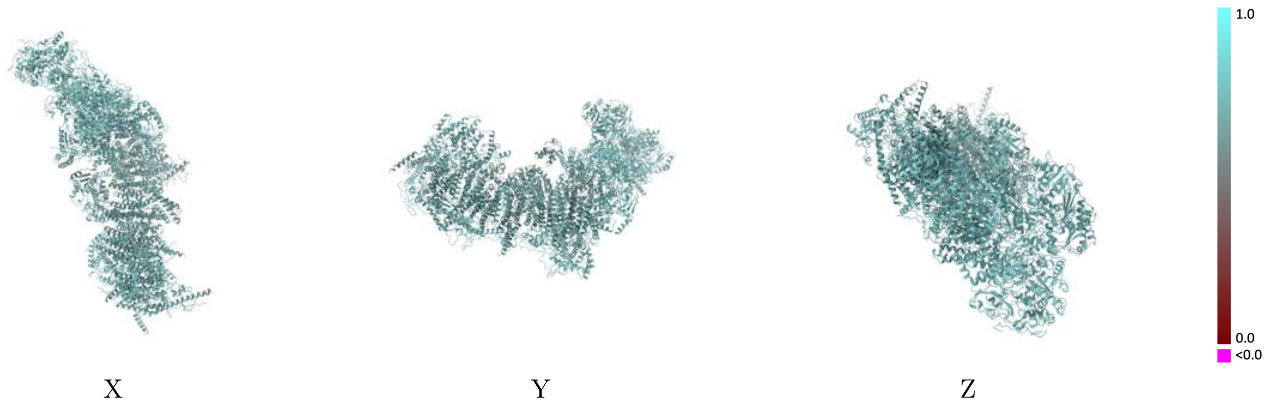
Y



Z

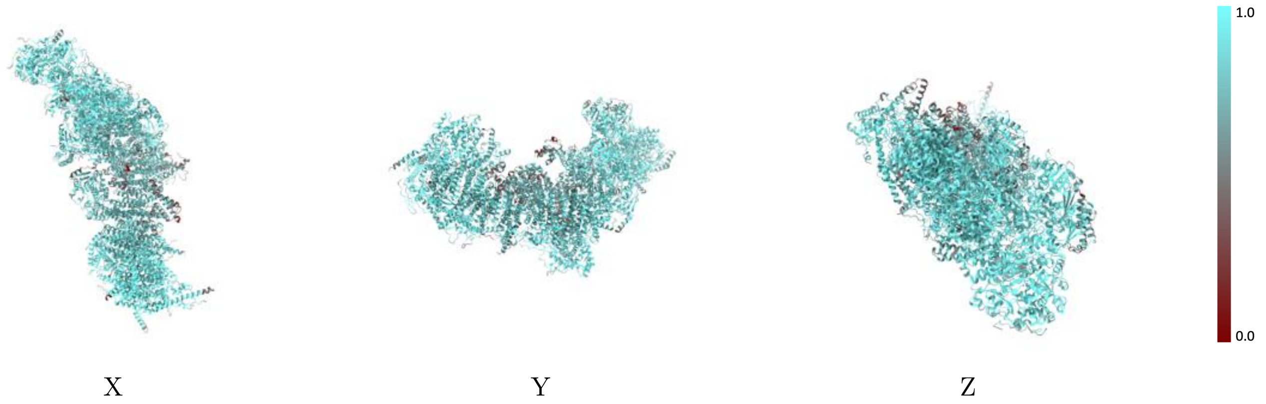
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



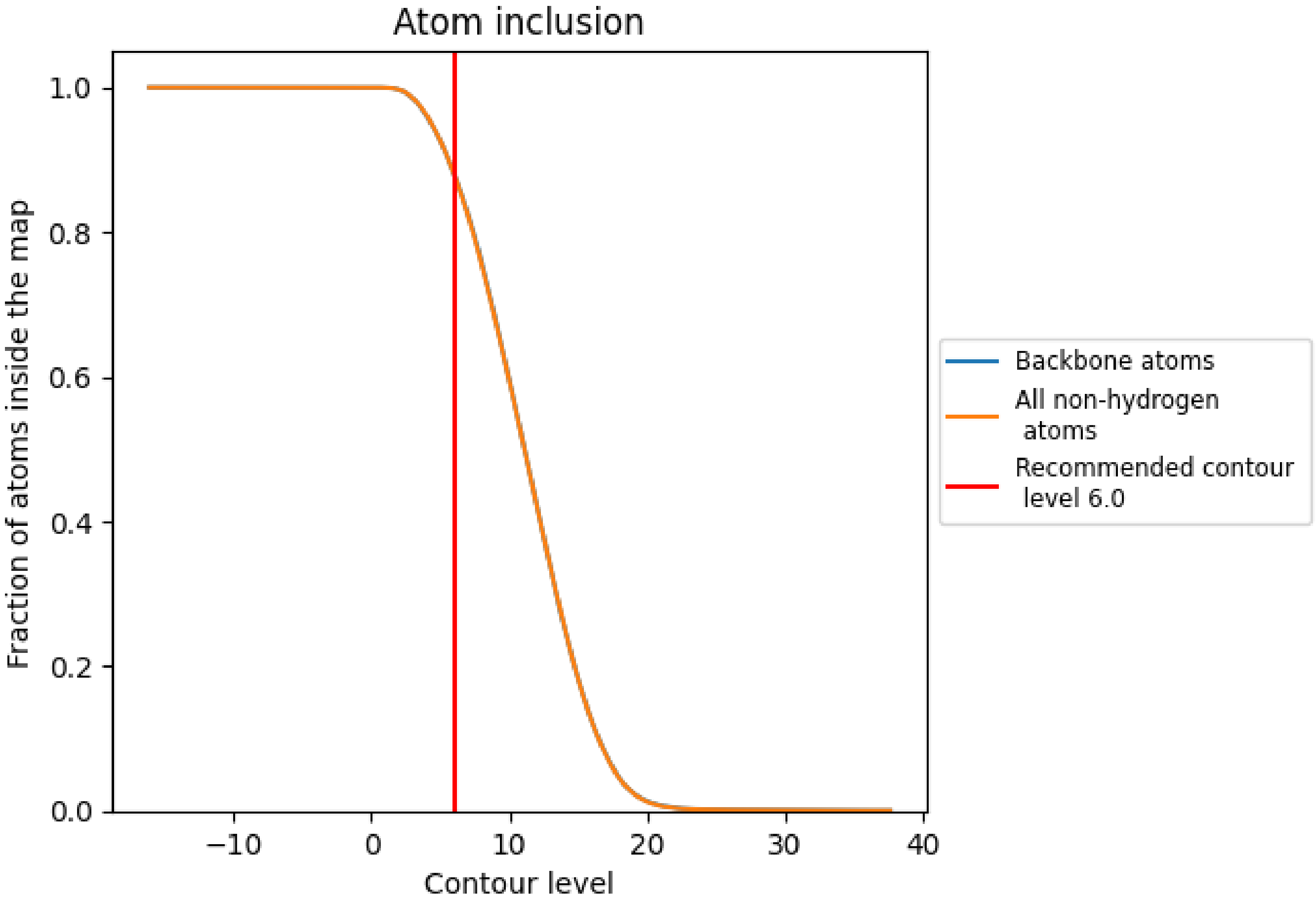
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8796	0.6960
A	0.8244	0.6800
B	0.9256	0.7230
C	0.9604	0.7340
D	0.9265	0.7280
E	0.8752	0.6910
F	0.9224	0.7050
G	0.9075	0.7120
H	0.9282	0.7010
I	0.9486	0.7370
J	0.7897	0.6740
K	0.8825	0.7000
L	0.9026	0.6870
M	0.9445	0.7060
N	0.9429	0.7130
O	0.8368	0.6710
P	0.8473	0.6950
Q	0.9084	0.7220
R	0.8850	0.7140
S	0.8065	0.6820
T	0.5901	0.6270
U	0.9340	0.6830
V	0.8527	0.7010
W	0.8631	0.7010
X	0.8491	0.6770
Y	0.5422	0.6420
Z	0.8339	0.6820
a	0.9445	0.6990
b	0.8107	0.6690
c	0.7374	0.6620
d	0.8571	0.6910
e	0.8273	0.6820
f	0.7489	0.6580
g	0.8741	0.6860
h	0.9004	0.6930

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Chain	Atom inclusion	Q-score
i	0.8743	0.6670
j	0.8885	0.6580
k	0.8682	0.6460
l	0.9002	0.6810
m	0.8297	0.6750
n	0.9197	0.6900
o	0.8781	0.6590
p	0.9114	0.6880
q	0.8447	0.7080
r	0.8787	0.7150
s	0.8563	0.6870